STIC Search Report
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STIC Database Tracking Number: 146737

TO:	From:
Ben Sackey Location: 5b31/5c18 Art Unit: 1626 Friday, March 11, 2005 Case Serial Number: 10/771926	Noble Jarrell Location: Biotech-Chem Library Rem 1B71 Phone: 272-2556 Noble.jarrell@uspto.gov

Search Notes

Noble

Access DB# 146737

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: BEN SACKEY Examiner #: 78489 Date: 3/3/05

Art Unit: 1626 Phone Number ~~308~~ 7-0704 Serial Number: 10/771,926

Mail Box and Bldg/Room Location: REM 5 831 Results Format Preferred (circle): (PAPER) DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

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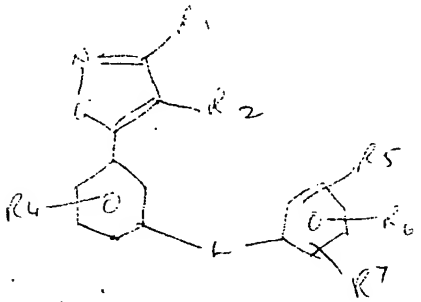
Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc. if known. Please attach a copy of the cover sheet, pertinent claims and abstract.

Title of Invention: Protein-tyrosine phosphatase inhibitors and uses thereof

Inventors (please provide full names): Zhili Xin et al.

Earliest Priority Filing Date: 2/14/03

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*



Example 23 is the elected species

R1 is as defined except hetcycles

R2 is hydrogen, alkyl, alkoxy, CN, OH, amino, hydroxyalkyl

R4 is hydrogen or alkyl

R5 is carboxyalkyl

R6 is hydroxy, hydroxyalkyl, amino

R7 is hydrogen, alkyl

L is C, J, K which consists of alkyl, alkenyl

X1-X2 = bond — X2 is -O-.

Thanks

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STAFF USE ONLY

Searcher: Noble

Searcher Phone #: —

Searcher Location: —

Date Searcher Picked Up: 3/11/05

Type of Search

NA Sequence (#) ____ AA Sequence (#) ____ Structure (#) 2 Bibliographic 1

Vendors and cost where applicable

STN 498

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Questel/Orbit ____

Dr.Link ____

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     FILE 'HCAPLUS' ENTERED AT 08:12:43 ON 11 MAR 2005
L1             1 US20040214870/PN
               E US2003-447407/AP,PRN
L2             1 US2003-447407P/AP,PRN
L3             1 L1-2

     FILE 'REGISTRY' ENTERED AT 08:13:32 ON 11 MAR 2005

     FILE 'HCAPLUS' ENTERED AT 08:13:33 ON 11 MAR 2005
L4               TRA L3 1- RN :       97 TERMS

     FILE 'REGISTRY' ENTERED AT 08:13:34 ON 11 MAR 2005
L5            97 SEA L4

     FILE 'WPIX' ENTERED AT 08:13:36 ON 11 MAR 2005
L6             1 US20040214870/PN
               E US2003-447407/AP,PRN
L7             2 (US2003-447407 OR US2003-447407P)/AP,PRN
L8             2 L6-7

=> b hcap
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FILE LAST UPDATED: 9 Mar 2005  (20050309/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> d all l3

L3   ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   2004:905629  HCAPLUS
DN   141:379917
ED   Entered STN:  29 Oct 2004
TI   Preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase
     (PTP1B) inhibitors.
IN   Xin, Zhili; Liu, Gang; Pei, Zhonghua; Szczepankiewicz, Bruce G.; Serby,
     Michael D.; Zhao, Hongyu
PA   USA
SO   U.S. Pat. Appl. Publ., 32 pp.
     CODEN: USXXCO
DT   Patent
LA   English
IC   ICM  A61K031-433
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ICS A61K031-426; A61K031-4245; A61K031-421; A61K031-4196; A61K031-4172
NCL 514362000; 514383000; 514381000; 514365000; 514374000; 514364000; 514396000; 548136000; 548143000; 548202000
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004214870	A1	20041028	US 2004-771926	20040204 <--
PRAI	US 2003-447407P	P	20030214 <--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2004214870	ICM	A61K031-433
	ICS	A61K031-426; A61K031-4245; A61K031-421; A61K031-4196; A61K031-4172
	NCL	514362000; 514383000; 514381000; 514365000; 514374000; 514364000; 514396000; 548136000; 548143000; 548202000
US 2004214870	ECLA	C07D261/18; C07D413/04+261+209C; C07D413/12+261+211 <--

OS MARPAT 141:379917
AB R1R2R3AB(R4)LCR5R6R7 [A = isoxazolyl, pyrazolyl, oxadiazolyl, triazolyl, isothiazolyl, imidazolyl, oxazolyl, tetrazolyl, thiadiazolyl; B, C = aryl, heterocyclyl; L = bond, GX1JX2K; G, J, K = bond, (substituted) alkyl, alkenyl, aryl, cycloalkyl; X1, X2 = bond, O, NRc, NRcCO, CO, NRcSO2; Rc = H, alkyl, aralkyl; R1 = alkyl, alkoxy, alkylsulfonyl, trifluoroalkylsulfonyl, alkylsulfonylaminoo, specified azolyl; R2-R7 = null, H, alkyl, alkylcarbonyl, alkoxy, alkoxyalkyl, aryl, arylcarbonyl, aralkyl, CO2H, halo, cyano, OH, hydroxylalkyl, NO2, trihaloalkyl, etc.; with provisos], were prepared Thus, Et 5-(tributylstannyl)isoxazole-3-carboxylate (preparation given), (E)-3-(3-iodophenyl)prop-2-en-1-ol (preparation given), tri-2-furylphosphine, tris(dibenzylideneacetone)dipalladium(0), and CuI were were stirred 30 min. in DMF to give Et 5-[3-[(1E)-3-hydroxyprop-1-enyl]phenyl]isoxazole-3-carboxylate. This was stirred with Me 2,6-dihydroxybenzoate, Ph3P, and di-Et azodicarboxylate in THF to give Et 5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylate. The latter was stirred with 2N NaOH in THF/MeOH to give 5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic acid. This inhibited PTP1B with Kic = 5.7 .mu.M.
ST arylisoxazolecarboxylate prepn protein tyrosine phosphatase inhibitor; isoxazolecarboxylate aryl prepn PTP1B inhibitor; inflammation cancer diabetes autoimmune disorder obesity treatment isoxazolecarboxylate prepn
IT Inflammation
(chronic, treatment; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Immune system
(immune system agents; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Diabetes mellitus
(insulin-dependent, treatment; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Diabetes mellitus
(non-insulin-dependent, treatment; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Anti-inflammatory agents
Antidiabetic agents
Antiobesity agents
Antitumor agents
Drug delivery systems
Human
(preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Osteoporosis
(treatment, antiosteoporotics; preparation of arylisoxazolecarboxylates as

protein-tyrosine phosphatase inhibitors)
IT Autoimmune disease
Neoplasm
Obesity
(treatment: preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT 745078-69-7P 745078-73-3P 745078-78-8P 745078-82-4P 745078-86-8P
745078-89-1P 745078-90-4P 745078-92-6P 745078-93-7P 745078-94-8P
745078-96-0P 745078-98-2P 745079-00-9P 745079-02-1P 745079-03-2P
745079-04-3P 745079-07-6P 745079-09-8P 745079-10-1P 745079-12-3P
745079-13-4P 745079-18-9P 745079-21-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT 50-99-7, Glucose, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(impaired glucose tolerance, treatment; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT 300865-11-6, Protein tyrosine phosphatase-1B
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT 74-89-5, Methylamine, reactions 75-36-5, Acetyl chloride 452-82-4, 4-Fluoro-3-iodotoluene 497-06-3, 3-Butene-1,2-diol 540-51-2, 2-Bromoethanol 553-90-2, Dimethyl oxalate 598-32-3, 3-Buten-2-ol 601-89-8, 2-Nitroresorcinol 616-25-1, 1-Penten-3-ol 626-01-7, 3-Iodoaniline 696-41-3, 3-Iodobenzaldehyde 867-13-0, Triethyl phosphonoacetate 994-89-8, Tributylstannylacetylene 1007-15-4 1664-54-6, 3-(3-Aminophenyl)propionic acid 2142-63-4, 3'-Bromoacetophenone 2150-45-0, Methyl 2,6-dihydroxybenzoate 3132-99-8, 3-Bromobenzaldehyde 10272-07-8 10365-98-7, 3-Methoxyphenylboronic acid 14337-43-0, Ethyl chlorooximidoacetate 14452-30-3, 3'-Iodoacetophenone 52415-29-9, 6-Bromoindole 54060-30-9, 3-Ethynylphenylamine 58313-23-8, Ethyl 3-iodobenzoate 95037-48-2, 1-Acetylpiperidine-4-carbonyl chloride hydrochloride 745079-28-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT 3147-50-0P 14367-96-5P 20950-56-5P, [1,1'-Biphenyl]-3,3',5-triol
25245-27-6P 30578-88-2P 33580-34-6P 68034-75-3P 68332-33-2P
73164-56-4P 81069-39-8P 83968-02-9P 93618-22-5P 119125-28-9P
126085-91-4P 141763-48-6P 185619-66-3P 227609-88-3P 281204-55-5P
745078-70-0P 745078-71-1P 745078-72-2P 745078-74-4P 745078-75-5P
745078-76-6P 745078-79-9P 745078-83-5P 745078-84-6P 745078-85-7P
745078-91-5P 745078-95-9P 745078-97-1P 745079-05-4P 745079-06-5P
745079-11-2P 745079-14-5P 745079-15-6P 745079-16-7P 745079-17-8P
745079-19-0P 745079-22-5P 745079-23-6P 745079-24-7P 745079-26-9P
745079-27-0P 745079-29-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)

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FOR DETAILS. <<<

=> d all l8 tot

L8 ANSWER 1 OF 2 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2004-774832 [76] WPIX
DNC C2004-271262
TI New carboxylic acid derivatives are protein tyrosine phosphatase-1B inhibitors useful for treating e.g. type I and II diabetes and impaired glucose tolerance.
DC B03
IN LIU, G; PEI, Z; SERBY, M D; SZCZEPANKIEWICZ, B G; XIN, Z; ZHAO, H
PA (LIUG-I) LIU G; (PEIZ-I) PEI Z; (SERB-I) SERBY M D; (SZCZ-I) SZCZEPANKIEWICZ B G; (XINZ-I) XIN Z; (ZHAO-I) ZHAO H
CYC 1
PI US 2004214870 A1 20041028 (200476)* 32 A61K031-433 <--
ADT US 2004214870 A1 **Provisional US 2003-447407P 20030214**, US 2004-771926 20040204
PRAI **US 2003-447407P 20030214**; US 2004-771926 20040204
IC ICM A61K031-433
ICS A61K031-4172; A61K031-4196; A61K031-421; A61K031-4245; A61K031-426
AB US2004214870 A UPAB: 20041125
NOVELTY - Carboxylic acid derivatives (I) and their salts and prodrugs are new.
DETAILED DESCRIPTION - Carboxylic acid derivatives of formula (I) and their salts and prodrugs are new.
A = 3-R1-4-R3-isoxazol-5-yl, 1-R2-3-R1-4-R3-1H-pyrazole-5-yl, 3-R1-4-R3-isothiazol-5-yl, 3-R1-(1,2,4)oxadiazol-5-yl, 1-R2-3-R1-(1,2,4)triazol-5-yl, 3-R1-(1,2,4)thiadiazol-5-yl, 2-R1-4-R2-4-R3-4H-imidazol-5-yl, 4-R3-5-R1-4H-(1,2,4)triazol-3-yl, 5-R1-(1,3,4)oxadiazol-2-yl, 3-methyl-5-R1-(1,3,4)thiadiazol-2-yl, 4-R2-4-R3-5-R1-4H-pyrazol-3-yl, 1-R3-2-R1-4-R2-1H-imidazol-5-yl, 2-R1-4-R2-oxazol-5-yl, 2-R1-4-R2-thiazol-5-yl, 5-R1-2H-tetrazol-2-yl, 3-R1-5-R2-1H-(1,2,4)triazol-1-yl, 4-R1-5-R3-1H-(1,2,3)triazol-1-yl or 2-R2-4-R1-5-R3-1H-imidazol-1-yl;
B' and C' = aryl or heterocycle;
R1 = alkyl, alkoxy, (trifluoro)alkyl-SO2, trifluoroalkyl-NH-, alkyl-SO2NH-, carboxy, cyano, HONH-carbonyl, RaONH-carbonyl, nitro, RaOC(O)-, HO3S-, H2NO2S-, RaNHO2S-, (HO)2(O)P-, (HO)2(O)PCH2-, (HO)2(O)PCHF-, (HO)2(O)PCF2-, 2H-tetrazol-5-yl, 3-hydroxyisoxazol-5-yl, 5-hydroxyisoxazol-3-yl, 3-hydroxypyrazol-5-yl, 2,2-dioxo-3H-(1,2,3,5)oxathiadiazol-4-yl, 2,2-dioxo-3H-(1,2,3,4)oxathiadiazol-5-yl, 3-hydroxy-(1,2,4)oxadiazol-5-yl, 3-hydroxy-(1,2,4)thiadiazol-5-yl, 2-hydroxy-(1,3,4)oxadiazol-5-yl, 2-mercapto-(1,3,4)oxadiazol-5-yl,

2-hydroxy-(1,3,4)thiadiazol-5-yl, 3-hydroxy-1H-(1,2,4)triazol-5-yl, 2-hydroxyoxazol-5-yl, 2-hydroxythiazol-5-yl, 2-oxo-1,3-dihydroimidazol-4-yl, 2,2-dioxo-3H-(1,2,3)oxathiazol-4-yl, 3-oxo-1,2-dihydro-(1,2,4)triazol-5-yl, 1-oxo-2,3-dihydro-(1,2,3,5)thiatriazol-4-yl, 2,4-dioxoimidazolidin-1-yl, 2,4-dioxothiazolidin-5-yl, 2,4-dioxooxazolidin-5-yl, 2-hydroxyoxazol-4-yl, 2,2-dioxo-3H-(1,2,3,4)oxathiadiazol-5-yl, 1,1-dioxo-2,3-dihydro-(1,2,3,5)thiatriazol-4-yl or 2,4-dioxoimidazolidin-5-yl:

R2 - R7 = absent, H, alkyl, alkylcarbonyl, alkoxy, alkoxyalkyl, alkoxycarbonyl, aryl, arylcarbonyl, arylalkyl, carboxy, carboxyalkyl, cyano, cycloalkyl, cycloalkylalkyl, halo, haloalkyl, heterocycle, heterocyclecarbonyl, heterocyclealkyl, hydroxy, hydroxyalkyl, nitro, trihaloalkyl, RaRbN, RaRbN-alkyl, RaRbN-carbonyl, RaRbN-carbonylalkyl, RaRbNN-sulfonyl, RaRbNN-sulfonylalkyl;

Ra and Rb = H, alkyl, alkoxycarbonyl, alkylcarbonyl, aryl, arylalkyl, cycloalkyl, cycloalkylalkyl, heterocycle or heterocyclealkyl;

L = G-X1-J-X2-K1- or bond;

G, J and K1 = alkyl, alkenyl, aryl or cycloalkyl (all optionally substituted by alkoxy, alkyl, halogen, hydroxy, hydroxyalkyl, carboxy or RdReN-) or bond;

Rd and Re = H, alkyl, alkoxycarbonyl, alkylcarbonyl or arylalkyl;

X1 and X2 = bond, -O-, -N(Rc)-, -N(Rc)C(O)-, -C(O)N(Rc)-, -N(Rc)S(O)2-, -S(O)2N(Rc)- and -C(O)-; and

Rc = H, alkyl or arylalkyl.

Provided that if J is absent then at least one of X1 and X2 must be absent.

ACTIVITY - Antidiabetic; Immunosuppressive; Antiinflammatory; Anorectic; Osteopathic; Cytostatic.

MECHANISM OF ACTION - Protein tyrosine phosphatase-1B inhibitor. 5-(3-((1E)-3-(3-hydroxy-2-(methoxycarbonyl)-phenoxy)prop-1-enyl)phenyl)isoxazole-3-carboxylic acid (Ia) was added to well containing pNPP in water. The reaction was initiated by adding diluted protein tyrosine phosphatase 1B and worked up. Results showed that (A) had Ki of 5.7 plus or minus 0.9.

USE - In pharmaceutical composition for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B e.g. type I and II diabetes, impaired glucose tolerance, insulin resistance, obesity, autoimmune disorders, acute and chronic inflammatory disorders, osteoporosis, cancer and malignant disorders (all claimed).

ADVANTAGE - (I) inhibits protein tyrosine phosphatase-1B.

Dwg.0/0

FS CPI
FA AB; GI; DCN
MC CPI: B05-B01E; B07-H; B14-C03; B14-D01E; B14-D07A; B14-E12; B14-F09; B14-G02D; B14-H01; B14-N01; B14-S04; N02-F; N07-D03

L8 ANSWER 2 OF 2 WPIX COPYRIGHT 2005 THE THOMSON CORP on STN
AN 2001-663337 [76] WPIX
DNN N2001-494250
TI An intravascular device which minimizes the possibility of emboli from the plaque entering the bloodstream by trapping it against the blood vessel wall.
DC P32
IN MULLER, P F; PATEL, U G; STACK, R S
PA (ADCA-N) ADVANCED CARDIOVASCULAR SYSTEM; (MULL-I) MULLER P F; (PATE-I) PATEL U G; (STAC-I) STACK R S
CYC 95
PI WO 2001082831 A2 20011108 (200176)* EN 32 A61F002-00
RW: AT BE CH CY DE DK EA ES FI FR GB GH GM GR IE IT KE LS LU MC MW MZ NL OA PT SD SE SL SZ TR TZ UG ZW
W: AE AG AL AM AT AU AZ BA BB BG BR BY BZ CA CH CN CO CR CU CZ DE DK DM DZ EE ES FI GB GD GE GH GM HR HU ID IL IN IS JP KE KG KP KR KZ LC LK LR LS LT LU LV MA MD MG MK MN MW MX MZ NO NZ PL PT RO RU SD SE SG SI SK SL TJ TM TR TT TZ UA UG UZ VN YU ZA ZW

AU 2001053475 A 20011112 (200222) A61F002-00
US 6592616 B1 20030715 (200348) A61F002-06
US 2003195556 A1 20031016 (200369) A61M029-00
ADT WO 2001082831 A2 WO 2001-US12152 20010412; AU 2001053475 A AU 2001-53475 20010412; US 6592616 B1 US 2000-560209 20000428; US 2003195556 A1 Cont of US 2000-560209 20000428. **US 2003-447407 20030529**
FDT AU 2001053475 A Based on WO 2001082831; US 2003195556 A1 Cont of US 6592616
PRAI US 2000-560209 20000428; **US 2003-447407 20030529**
IC ICM A61F002-00; A61F002-06; A61M029-00
AB WO 200182831 A UPAB: 20011227
NOVELTY - An intravascular device (10) comprises a permanently implantable tubular net (12) made from a flexible, blood permeable and biocompatible material. An expandable member (20) is attached to each end of the net and is capable of expanding to contact the wall of the blood vessel to maintain the net over the plaque.

DETAILED DESCRIPTION - INDEPENDENT CLAIMS are also included for the following:

(a) a catheter for delivering a stent and a plaque-trapping device into a blood vessel, comprising an inner member having an expandable contracted stent and a collapsed plaque-trapping device, and a retractable restraining sheath overlying the inner member and axially movable w.r.t. to it;

(b) a system for treating an area of plaque in a blood vessel comprising the plaque-trapping device, an implantable stent and a delivery catheter;

(c) a method of treating an area of plaque in a blood vessel;

(d) and a further intravascular device containing a means for maintaining a set longitudinal distance between the expandable members.

USE - The device is used to trap an area of plaque against the wall of a blood vessel (claimed) during e.g. a balloon angioplasty or stenting procedure. It is particularly useful for procedures in critical arteries such as carotid arteries, where blockages must be avoided.

ADVANTAGE - The device minimizes the possibility of emboli from the plaque entering the bloodstream (claimed). It is not necessary to employ a filtering device to catch and remove debris in the bloodstream.

DESCRIPTION OF DRAWING(S) - The drawing shows a perspective view of the plaque-trapping device.

plaque-trapping device; 10
tubular net; 12
proximal end; 14
distal end; 16
inner lumen; 18
expandable member; 20
longitudinal strut. 22

Dwg.1/14
FS GMPI
FA AB; GI

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     FILE 'HCAPLUS' ENTERED AT 08:12:43 ON 11 MAR 2005
L1             1 US20040214870/PN
                 E US2003-447407/AP.PRN
L2             1 US2003-447407P/AP.PRN
L3             1 L1-2

     FILE 'REGISTRY' ENTERED AT 08:13:32 ON 11 MAR 2005

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L4               TRA L3 1- RN :       97 TERMS

     FILE 'REGISTRY' ENTERED AT 08:13:34 ON 11 MAR 2005
L5            97 SEA L4

     FILE 'WPIX' ENTERED AT 08:13:36 ON 11 MAR 2005
L6             1 US20040214870/PN
                 E US2003-447407/AP,PRN
L7             2 (US2003-447407 OR US2003-447407P)/AP,PRN
L8             2 L6-7

     FILE 'REGISTRY' ENTERED AT 08:27:41 ON 11 MAR 2005
L9               STR
L10            1 L9
L11           52 L9 FULL
L12              STR L9
L13            0 L12
L14           34 L12 FULL
                 SAV TEM L11 SAC926F0/A
                 SAV TEM L14 SAC926F1/A

     FILE 'HCAPLUS' ENTERED AT 08:38:27 ON 11 MAR 2005
L15           15 L11 OR L14
                 SEL AN 1-3 L15
L16            3 E1-6 AND L15
L17           12 L15 NOT L16

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Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html
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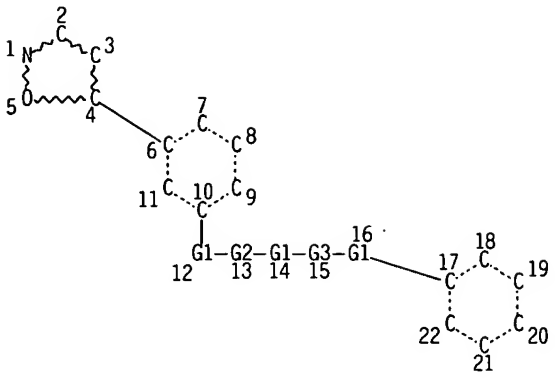
L9 STR



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VAR G3=O/N/23-14 24-16/24-14 23-16/26-14 27-16/27-14 26-16/28
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 17 10 4
NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE
L11 52 SEA FILE=REGISTRY SSS FUL L9

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SEARCH TIME: 00.00.01

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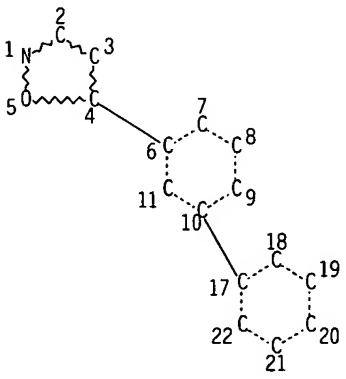
L12 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 17 10 4

NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L14 34 SEA FILE=REGISTRY SSS FUL L12

100.0% PROCESSED 2387 ITERATIONS 34 ANSWERS
SEARCH TIME: 00.00.01

=> b hcap
FILE 'HCAPLUS' ENTERED AT 08:42:19 ON 11 MAR 2005
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FILE COVERS 1907 - 11 Mar 2005 VOL 142 ISS 11
FILE LAST UPDATED: 9 Mar 2005 (20050309/ED)

This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d all fhitstr l16 tot

L16 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
AN **2004:905629** HCAPLUS
DN 141:379917
ED Entered STN: 29 Oct 2004
TI Preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase (PTP1B) inhibitors.
IN Xin, Zhili; Liu, Gang; Pei, Zhonghua; Szczepankiewicz, Bruce G.; Serby, Michael D.; Zhao, Hongyu
PA USA
SO U.S. Pat. Appl. Publ., 32 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM A61K031-433
ICS A61K031-426; A61K031-4245; A61K031-421; A61K031-4196; A61K031-4172
NCL 514362000; 514383000; 514381000; 514365000; 514374000; 514364000; 514396000; 548136000; 548143000; 548202000
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2004214870	A1	20041028	US 2004-771926	20040204
PRAI US 2003-447407P	P	20030214		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2004214870	ICM	A61K031-433

ICS A61K031-426; A61K031-4245; A61K031-421; A61K031-4196; A61K031-4172
NCL 514362000; 514383000; 514381000; 514365000; 514374000; 514364000; 514396000; 548136000; 548143000; 548202000
US 2004214870 ECLA C07D261/18; C07D413/04+261+209C; C07D413/12+261+211
OS MARPAT 141:379917
AB R1R2R3AB(R4)LCR5R6R7 [A = isoxazolyl, pyrazolyl, oxadiazolyl, triazolyl, isothiazolyl, imidazolyl, oxazolyl, tetrazolyl, thiadiazolyl; B, C = aryl, heterocyclyl; L = bond, GX1JX2K; G, J, K = bond, (substituted) alkyl, alkenyl, aryl, cycloalkyl; X1, X2 = bond, O, NRc, NRcCO, CO, NRcSO2; Rc = H, alkyl, aralkyl; R1 = alkyl, alkoxy, alkylsulfonyl, trifluoroalkylsulfonyl, alkylsulfonylaminoo, specified azolyl; R2-R7 = null, H, alkyl, alkylcarbonyl, alkoxy, alkoxyalkyl, aryl, arylcarbonyl, aralkyl, CO2H, halo, cyano, OH, hydroxylalkyl, NO2, trihaloalkyl, etc.; with provisos], were prepared Thus, Et 5-(tributylstannyl)isoxazole-3-carboxylate (preparation given), (E)-3-(3-iodophenyl)prop-2-en-1-ol (preparation given), tri-2-furylphosphine, tris(dibenzylideneacetone)dipalladium(0), and CuI were were stirred 30 min. in DMF to give Et 5-[3-[(1E)-3-hydroxyprop-1-enyl]phenyl]isoxazole-3-carboxylate. This was stirred with Me 2,6-dihydroxybenzoate, Ph3P, and di-Et azodicarboxylate in THF to give Et 5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylate. The latter was stirred with 2N NaOH in THF/MeOH to give 5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic acid. This inhibited PTP1B with Kic = 5.7 .mu.M.
ST arylisoxazolecarboxylate prepn protein tyrosine phosphatase inhibitor; isoxazolecarboxylate aryl prepn PTP1B inhibitor; inflammation cancer diabetes autoimmune disorder obesity treatment isoxazolecarboxylate prepn
IT Inflammation
(chronic, treatment; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Immune system
(immune system agents; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Diabetes mellitus
(insulin-dependent, treatment; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Diabetes mellitus
(non-insulin-dependent, treatment; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Anti-inflammatory agents
Antidiabetic agents
Antiobesity agents
Antitumor agents
Drug delivery systems
Human
(preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Osteoporosis
(treatment, antiosteoporotics; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT Autoimmune disease
Neoplasm
Obesity
(treatment; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)
IT 745078-69-7P 745078-73-3P **745078-78-8P** 745078-82-4P
745078-86-8P 745078-89-1P 745078-90-4P 745078-92-6P
745078-93-7P **745078-94-8P** 745078-96-0P 745078-98-2P
745079-00-9P 745079-02-1P 745079-03-2P 745079-04-3P 745079-07-6P
745079-09-8P 745079-10-1P 745079-12-3P 745079-13-4P 745079-18-9P
745079-21-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES

(Uses)
(claimed compound; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)

IT 50-99-7, Glucose, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(impaired glucose tolerance, treatment; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)

IT 300865-11-6, Protein tyrosine phosphatase-1B
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(inhibitors; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)

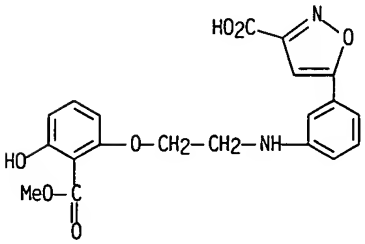
IT 74-89-5, Methylamine, reactions 75-36-5, Acetyl chloride 452-82-4, 4-Fluoro-3-iodotoluene 497-06-3, 3-Butene-1,2-diol 540-51-2, 2-Bromoethanol 553-90-2, Dimethyl oxalate 598-32-3, 3-Buten-2-ol 601-89-8, 2-Nitroresorcinol 616-25-1, 1-Penten-3-ol 626-01-7, 3-Iodoaniline 696-41-3, 3-Iodobenzaldehyde 867-13-0, Triethyl phosphonoacetate 994-89-8, Tributylstannylacetylene 1007-15-4 1664-54-6, 3-(3-Aminophenyl)propionic acid 2142-63-4, 3'-Bromoacetophenone 2150-45-0, Methyl 2,6-dihydroxybenzoate 3132-99-8, 3-Bromobenzaldehyde 10272-07-8 10365-98-7, 3-Methoxyphenylboronic acid 14337-43-0, Ethyl chlorooximidoacetate 14452-30-3, 3'-Iodoacetophenone 52415-29-9, 6-Bromoindole 54060-30-9, 3-Ethynylphenylamine 58313-23-8, Ethyl 3-iodobenzoate 95037-48-2, 1-Acetylpiperidine-4-carbonyl chloride hydrochloride 745079-28-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)

IT 3147-50-0P 14367-96-5P 20950-56-5P, [1,1'-Biphenyl]-3,3',5-triol 25245-27-6P 30578-88-2P 33580-34-6P 68034-75-3P 68332-33-2P 73164-56-4P 81069-39-8P 83968-02-9P 93618-22-5P 119125-28-9P 126085-91-4P 141763-48-6P 185619-66-3P 227609-88-3P 281204-55-5P 745078-70-0P 745078-71-1P 745078-72-2P 745078-74-4P 745078-75-5P 745078-76-6P 745078-79-9P 745078-83-5P 745078-84-6P 745078-85-7P 745078-91-5P **745078-95-9P** 745078-97-1P 745079-05-4P 745079-06-5P 745079-11-2P 745079-14-5P 745079-15-6P 745079-16-7P 745079-17-8P 745079-19-0P 745079-22-5P 745079-23-6P 745079-24-7P 745079-26-9P 745079-27-0P 745079-29-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)

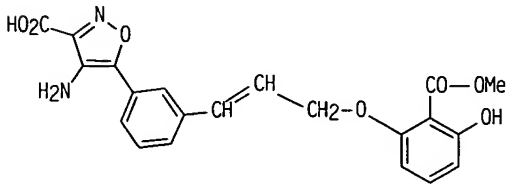
IT **745078-78-8P**
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of arylisoxazolecarboxylates as protein-tyrosine phosphatase inhibitors)

RN 745078-78-8 HCAPLUS

CN 3-Isoxazolecarboxylic acid, 5-[3-[[2-[3-hydroxy-2-(methoxycarbonyl)phenoxy]ethyl]amino]phenyl]- (9CI) (CA INDEX NAME)



L16 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
AN **2004:863100** HCAPLUS
DN 142:232
ED Entered STN: 19 Oct 2004
TI Isoxazole carboxylic acids as protein tyrosine phosphatase 1B (PTP1B) inhibitors
AU Zhao, Hongyu; Liu, Gang; Xin, Zhili; Serby, Michael D.; Pei, Zhonghua; Szczepankiewicz, Bruce G.; Hajduk, Philip J.; Abad-Zapatero, Cele; Hutchins, Charles W.; Lubben, Thomas H.; Ballaron, Stephen J.; Haasch, Deanna L.; Kaszubska, Wiweka; Rondinone, Cristina M.; Trevillyan, James M.; Jirousek, Michael R.
CS Metabolic Disease Research, Global Pharmaceutical Research and Development, Abbott Laboratories, Abbott Park, IL, 60064-6098, USA
SO Bioorganic & Medicinal Chemistry Letters (2004), 14(22), 5543-5546
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier B.V.
DT Journal
LA English
CC 1-3 (Pharmacology)
Section cross-reference(s): 28
GI



I

AB Guided by X-ray crystallog., we have extended the structure-activity relationship (SAR) study on an isoxazole carboxylic acid-based PTP1B inhibitor and more potent and equally selective (>20-fold selectivity over the highly homologous T-cell PTPase, TCPTP) PTP1B inhibitors were identified. Inhibitor I demonstrated good cellular activity against PTP1B in COS 7 cells.

ST isoxazole carboxylate prepn protein tyrosine phosphatase inhibitor structure

IT Structure-activity relationship
(isoxazole carboxylic acids as protein tyrosine phosphatase 1B inhibitors)

IT 300865-11-6, Protein tyrosine phosphatase 1B
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(isoxazole carboxylic acids as protein tyrosine phosphatase 1B inhibitors)

IT 745079-13-4P 745079-21-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(isoxazole carboxylic acids as protein tyrosine phosphatase 1B inhibitors)

IT **745078-78-8** 745078-92-6 **794525-51-2** 794525-52-3 794525-53-4
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(isoxazole carboxylic acids as protein tyrosine phosphatase 1B inhibitors)

IT 2150-45-0, Methyl 2,6-dihydroxybenzoate 14337-43-0, Ethyl chlorooximido

acetate 74141-12-1 745079-22-5 794525-54-5
RL: RCT (Reactant): RACT (Reactant or reagent)
(isoxazole carboxylic acids as protein tyrosine phosphatase 1B inhibitors)
IT 745079-16-7P 745079-17-8P 745079-23-6P 745079-26-9P 745079-27-0P
745079-29-2P 794525-55-6P 794525-56-7P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(isoxazole carboxylic acids as protein tyrosine phosphatase 1B inhibitors)
RE.CNT 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Barford, D; Science 1994, V263, P1397 HCAPLUS
(2) Cheng, A; Eur J Biochem 2002, V269, P1050 HCAPLUS
(3) Elchebly, M; Science 1999, V283, P1544 HCAPLUS
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(16) Protein Data Bank; www.rcsb.org
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(22) Wierenga, W; J Org Chem 1979, V44, P310 HCAPLUS
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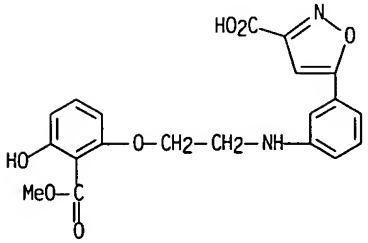
(25) Zhang, Z; Expert Opin Investig Drug 2003, V12, P223 HCAPLUS
(26) Zinker, B; Proc Natl Acad Sci U S A 2002, V99, P11357 HCAPLUS
IT **745078-78-8**
RL: PAC (Pharmacological activity): THU (Therapeutic use): BIOL (Biological study): USES (Uses)
(isoxazole carboxylic acids as protein tyrosine phosphatase 1B inhibitors)
RN 745078-78-8 HCAPLUS
CN 3-Isoxazolecarboxylic acid, 5-[3-[[2-[3-hydroxy-2-(methoxycarbonyl)phenoxy]ethyl]amino]phenyl]- (9CI) (CA INDEX NAME)



L16 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
AN **2004:701813** HCAPLUS
DN 141:225493
ED Entered STN: 27 Aug 2004

TI Preparation of arylazole derivatives as protein-tyrosine phosphatase inhibitors
IN Xin, Zhili; Liu, Gang; Pei, Zhonghua; Szczepankiewicz, Bruce G.; Serby, Michael D.; Zhao, Hongyu
PA USA
SO U.S. Pat. Appl. Publ., 32 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM A61K031-675
ICS A61K031-433
NCL 514363000; 514364000; 514365000; 514374000; 514381000; 514396000; 514406000; 514079000; 548112000; 548128000
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 7
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2004167188	A1	20040826	US 2003-366830	20030214
PRAI US 2003-366830		20030214		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2004167188	ICM	A61K031-675
	ICS	A61K031-433
	NCL	514363000; 514364000; 514365000; 514374000; 514381000; 514396000; 514406000; 514079000; 548112000; 548128000
US 2004167188	ECLA	C07D261/18; C07D413/04+261+209C; C07D413/12+261+211

OS MARPAT 141:225493
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The present invention is directed to compds. of formula (I), or pharmaceutically suitable salts or prodrugs thereof [wherein A = Q-Q16; B, C = aryl, heterocycle; R1 = alkyl, alkoxy, alkylsulfonyl, trifluoroalkylsulfonyl, trifluoroalkylamino, alkylsulfamoyl, CO2H or its ester, cyano, N-hydroxycarbamoyl or its ether, nitro, HO3S, (un)substituted sulfamoyl, (HO)2(O)P, (HO)2(O)PCH2, (HO)2(O)PCHF, (HO)2(O)PCF2, heterocycle; R2-R7 = H, alkyl, alkylcarbonyl, alkoxy, alkoxyalkyl, alkoxycarbonyl, aryl, arylcarbonyl, arylalkyl, carboxy, carboxyalkyl, cyano, cycloalkyl, cycloalkylalkyl, halo, haloalkyl, heterocycle, heterocyclecarbonyl, heterocyclealkyl, hydroxy, hydroxyalkyl, nitro, trihaloalkyl, each (un)substituted NH2, CONH2, or SO2NH2, etc.; L = -G-X1-J-X2-K- or a bond; G, J, K = a bond, each (un)substituted alkyl, alkenyl, aryl, or cycloalkyl; X1, X2 = a bond, O, N(Rc), N(Rc)CO, C(O)N(Rc), N(Rc)S(O)2, S(O)2N(Rc), C(O); wherein Rc = H, alkyl, arylalkyl; provided that if J is absent, then at least one of X1 and X2 must be absent]. These compds. are useful for the selective inhibition of protein tyrosine phosphatase-1B (PTP1B), and are useful for the treatment of disorders caused by overexpressed or altered protein tyrosine phosphatase 1B, i.e. (1) type I and type II diabetes, impaired glucose tolerance and insulin resistance, (2) obesity, and (3) autoimmune disorders, acute and chronic inflammatory disorders, osteoporosis, cancer, and malignant disorders. Thus, Et 5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylate > [0172]. Etherification of Et 5-[3-((1E)-3-hydroxyprop-1-enyl)phenyl]isoxazole-3-carboxylate with Me 2,6-dihydroxybenzoate using triphenylphosphine and di-Et azodicarboxylate in THF at ambient temperature for 30 min gave Et 5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylate which was dissolved in THF/MeOH,

stirred with 2 N aqueous NaOH for 10 min, and acidified with 1 N aqueous HCl to give 5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic acid (II). II showed phosphatase inhibition consts. (Ki) of 5.7.+-.0.9, 201.6.+-.26.5, and >300 .mu.M against protein tyrosine phosphatase-1B, T-Cell protein tyrosine phosphatase (TC-PTP), and SHP-2 phosphatase, resp.

ST phenylisoxazole prepn protein tyrosine phosphatase inhibitor; arylazole prepn protein tyrosine phosphatase inhibitor; diabetes treatment phenylisoxazole prepn; impaired glucose tolerance treatment phenylisoxazole prepn; insulin resistance treatment phenylisoxazole prepn; obesity treatment phenylisoxazole prepn; autoimmune disorder treatment phenylisoxazole prepn; inflammatory disorder treatment phenylisoxazole prepn; osteoporosis treatment phenylisoxazole prepn; cancer treatment phenylisoxazole prepn

IT Inflammation
(acute; preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)

IT Inflammation
(chronic; preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)

IT Diabetes mellitus
(insulin-dependent; preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)

IT Diabetes mellitus
(non-insulin-dependent; preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)

IT Anti-inflammatory agents
Antidiabetic agents
Antiobesity agents
Antitumor agents
Autoimmune disease
Neoplasm
Obesity
Osteoporosis
(preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)

IT Bone
(resorption, inhibitors; preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)

IT 50-99-7, D-Glucose, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(impaired glucose tolerance; preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)

IT 14367-96-5P, 1-(3-Bromophenyl)-2-nitroethanone 20950-56-5P, 3,5,3'-Trihydroxybiphenyl 25245-27-6P, 3,5-Dimethoxyiodobenzene 30578-88-2P, Methyl 2,6-dihydroxy-3-nitrobenzoate 33580-34-6P, 3,5,3'-Trimethoxybiphenyl 52234-79-4P, N-Methyl-2,6-dihydroxybenzamide 68034-75-3P, 3-(3-Iodophenyl)propionic Acid 68332-33-2P, Ethyl 3-(3-iodophenyl)-3-oxopropanoate 73164-56-4P, N-(2,6-Dihydroxyphenyl)acetamide 81069-39-8P, Ethyl (2E)-3-(3-iodophenyl)-2-propenoate 83968-02-9P, 2,2-Dimethyl-4-vinyl-1,3-dioxolane 93618-22-5P, Methyl 4-(3-bromophenyl)-2,4-dioxobutanoate 119125-28-9P, 1-[(tert-Butyldimethylsilyl)oxy]but-3-en-2-ol 126085-91-4P, Ethyl 5-(tributylstannyl)isoxazole-3-carboxylate 141763-48-6P, 3-(3-Iodophenyl)-1-propanol 185619-66-3P, (3-Ethynylphenyl)carbamic Acid tert-Butyl Ester 227609-88-3P, 4-Fluoro-3-iodobenzaldehyde 260050-97-3P, 4-Fluoro-3-iodobenzyl bromide 281204-55-5P,

2-(6-Bromo-1H-indol-1-yl)ethanol 609848-44-4P, Methyl 5-(3-iodophenyl)isoxazole-3-carboxylate 745078-70-0P, (2E)-3-(3-Iodophenyl)prop-2-en-1-ol 745078-71-1P, Ethyl 5-[3-((1E)-3-hydroxyprop-1-enyl)phenyl]isoxazole-3-carboxylate 745078-72-2P, Ethyl 5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylate 745078-74-4P, 5-(3-Bromophenyl)isoxazole-3-carboxylic Acid Methyl Ester 745078-75-5P, 5-[3-(3-Oxobutyl)phenyl]isoxazole-3-carboxylic Acid Methyl Ester 745078-76-6P, Methyl 5-[3-(3-hydroxybutyl)phenyl]isoxazole-3-carboxylate 745078-77-7P, Methyl 5-[3-[3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]butyl]phenyl]isoxazole-3-carboxylate 745078-79-9P, 2-[(3-Iodophenyl)amino]ethanol 745078-80-2P, Methyl 2-hydroxy-6-[2-[(3-iodophenyl)amino]ethoxy]benzoate **745078-81-3P**, Ethyl 5-[3-[[2-[3-hydroxy-2-(methoxycarbonyl)phenoxy]ethyl]amino]phenyl]isoxazole-3-carboxylate 745078-83-5P, 5-(3-tert-Butoxycarbonylaminophenyl)isoxazole-3-carboxylic acid Ethyl Ester 745078-84-6P, Ethyl 5-(3-aminophenyl)isoxazole-3-carboxylate 745078-85-7P, Ethyl 5-[3-[[(1-acetylpiperidin-4-yl)carbonyl]amino]phenyl]isoxazole-3-carboxylate 745078-87-9P, 2-Hydroxy-6-[2-[(3-iodophenyl)amino]ethoxy]-N-methylbenzamide **745078-88-0P**, Ethyl 5-[3-[[2-[3-hydroxy-2-[(methylamino)carbonyl]phenoxy]ethyl]amino]phenyl]isoxazole-3-carboxylate 745078-91-5P, 5-[3-(3-Hydroxypropyl)phenyl]isoxazole-3-carboxylic Acid Ethyl Ester **745078-95-9P**, Methyl 5-[3'-[3-(methoxycarbonyl)isoxazol-5-yl]-1,1'-biphenyl-3-yl]isoxazole-3-carboxylate 745078-97-1P, Ethyl (1R,2R)-2-(3-iodophenyl)cyclopropanecarboxylate 745078-99-3P, Methyl 5-(3-bromo-4-methoxyphenyl)isoxazole-3-carboxylate 745079-01-0P, Methyl 5-(3-bromo-4-fluorophenyl)isoxazole-3-carboxylate 745079-05-4P, Methyl 2-[[1-[[(tert-butyldimethylsilyl)oxy]methyl]prop-2-enyl]oxy]-6-hydroxybenzoate 745079-06-5P, Methyl 5-[3-[(1E)-4-[(tert-butyldimethylsilyl)oxy]-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]but-1-enyl]phenyl]isoxazole-3-carboxylate 745079-08-7P, Ethyl 5-[1-(2-hydroxyethyl)-1H-indol-6-yl]isoxazole-3-carboxylate 745079-11-2P, N-Benzyl-2,6-dihydroxybenzamide 745079-14-5P, Ethyl 5-(3-bromophenyl)-4-nitroisoxazole-3-carboxylate 745079-15-6P, Ethyl 4-amino-5-(3-bromophenyl)isoxazole-3-carboxylate 745079-16-7P, Ethyl 4-amino-5-[3-((1E)-3-hydroxyprop-1-enyl)phenyl]isoxazole-3-carboxylate 745079-17-8P, Ethyl 4-amino-5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylate 745079-19-0P, 3,5,3'-Trihydroxybiphenyl-4-carboxylic Acid Methyl Ester 745079-22-5P, tert-Butyl 3-(3-iodophenyl)-3-oxopropanoate 745079-23-6P 745079-24-7P, Ethyl 4-(hydroxymethyl)-5-(3-iodophenyl)isoxazole-3-carboxylate 745079-25-8P 745079-26-9P, Ethyl 4-[(acetyloxy)methyl]-5-(3-iodophenyl)isoxazole-3-carboxylate 745079-27-0P, Ethyl 4-[(acetyloxy)methyl]-5-[3-((1E)-3-hydroxyprop-1-enyl)phenyl]isoxazole-3-carboxylate 745079-29-2P, Ethyl 4-[(acetyloxy)methyl]-5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)

IT 300865-11-6, Protein tyrosine phosphatase 1B

RL: BSU (Biological study, unclassified); BIOL (Biological study)

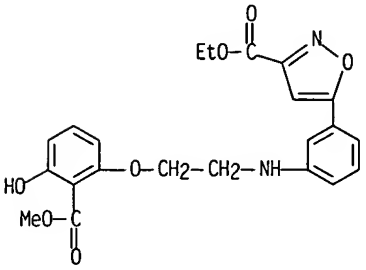
(preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)

IT 745078-69-7P, 5-[3-[(1E)-3-[3-Hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic Acid 745078-73-3P, 5-[3-[3-[3-Hydroxy-2-(methoxycarbonyl)phenoxy]butyl]phenyl]isoxazole-3-carboxylic Acid **745078-78-8P**, 5-[3-[[2-[3-Hydroxy-2-(methoxycarbonyl)phenoxy]ethyl]amino]phenyl]isoxazole-3-carboxylic Acid 745078-82-4P, 5-[3-[[(1-Acetylpiperidin-4-yl)carbonyl]amino]phenyl]isoxazo

le-3-carboxylic Acid **745078-86-8P**, 5-[3-[[2-[3-Hydroxy-2-[(methylamino)carbonyl]phenoxy]ethyl]amino]phenyl]isoxazole-3-carboxylic Acid 745078-89-1P, 5-[3-[(1E)-3-[3-Hydroxy-2-[(methylamino)carbonyl]phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic Acid 745078-90-4P, 5-[3-[3-[3-Hydroxy-2-(methoxycarbonyl)phenoxy]propyl]phenyl]isoxazole-3-carboxylic Acid 745078-92-6P, 5-[2-Fluoro-5-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic Acid 745078-93-7P, 5-[3-[(1E)-3-(3-Hydroxy-2-nitrophenoxy)prop-1-enyl]phenyl]isoxazole-3-carboxylic Acid **745078-94-8P**, 5-[3'-[3-(Carboxy)isoxazol-5-yl]-1,1'-biphenyl-3-yl]isoxazole-3-carboxylic Acid 745078-96-0P, 5-[3-[(1S,2S)-2-[[3-Hydroxy-2-(methoxycarbonyl)phenoxy]methyl]cyclopropyl]phenyl]isoxazole-3-carboxylic Acid 745078-98-2P, 5-[3-[3-[3-Hydroxy-2-(methoxycarbonyl)phenoxy]butyl]-4-methoxyphenyl]isoxazole-3-carboxylic Acid 745079-00-9P, 5-[4-Fluoro-3-[3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]butyl]phenyl]isoxazole-3-carboxylic Acid 745079-02-1P, 5-[3-[3-[3-Hydroxy-2-(methoxycarbonyl)phenoxy]pentyl]phenyl]isoxazole-3-carboxylic Acid 745079-03-2P, 5-[3-[(1E)-3-(3-Hydroxy-2-propionylphenoxy)prop-1-enyl]phenyl]isoxazole-3-carboxylic Acid 745079-04-3P, 5-[3-[(1E)-4-Hydroxy-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]but-1-enyl]phenyl]isoxazole-3-carboxylic Acid 745079-07-6P, 5-[1-[2-[3-Hydroxy-2-(methoxycarbonyl)phenoxy]ethyl]-1H-indol-6-yl]isoxazole-3-carboxylic Acid 745079-09-8P, 5-[3-[(1E)-3-[2-(Acetylamino)-3-hydroxyphenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic Acid 745079-10-1P, 5-[3-[(1E)-3-[2-[(Benzylamino)carbonyl]-3-hydroxyphenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic Acid 745079-12-3P, 5-[3-[(1E)-3-[3-Hydroxy-2-(methoxycarbonyl)-4-nitrophenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic Acid 745079-13-4P, 4-Amino-5-[3-[(1E)-3-[3-hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic Acid 745079-18-9P, 5-[3-[(1E)-3-[[3',5-Dihydroxy-4-(methoxycarbonyl)-1,1'-biphenyl-3-yl]oxy]prop-1-enyl]phenyl]isoxazole-3-carboxylic Acid 745079-20-3P, 5-[3-[3-[(5,3'-Dihydroxy-4-methoxycarbonylbiphenyl-3-yl)oxy]-2-propenyl]phenyl]isoxazole-3-carboxylic Acid 745079-21-4P, 5-[3-[(1E)-3-[3-Hydroxy-2-(methoxycarbonyl)phenoxy]prop-1-enyl]phenyl]-4-(hydroxymethyl)isoxazole-3-carboxylic Acid
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)

IT 74-89-5, Methylamine, reactions 75-36-5, Acetyl chloride 75-65-0, tert-Butanol, reactions 77-76-9, 2,2-Dimethoxypropane 100-46-9, Benzylamine, reactions 107-18-6, Allyl alcohol, reactions 452-82-4, 4-Fluoro-3-iodotoluene 497-06-3, 3-Butene-1,2-diol 540-51-2, 2-Bromoethanol 553-90-2, Dimethyl oxalate 601-89-8, 2-Nitroresorcinol 616-25-1, 1-Penten-3-ol 626-01-7, 3-Iodoaniline 688-73-3, Tributyltin 696-41-3, 3-Iodobenzaldehyde 867-13-0, Triethyl phosphonoacetate 1007-15-4, 3'-Bromo-4'-fluoroacetophenone 1664-54-6, 3-(3-Aminophenyl)propionic acid 2142-63-4, 3'-Bromoacetophenone 2150-45-0, Methyl 2,6-dihydroxybenzoate 3132-99-8, 3-Bromobenzaldehyde 3361-72-6, 1-(2,6-Dihydroxyphenyl)propanone 5470-11-1 10272-07-8, 3,5-Dimethoxyaniline 10365-98-7, 3-Methoxyphenylboronic acid 14337-43-0, Ethyl chlorooximidoacetate 14452-30-3, 3'-Iodoacetophenone 18162-48-6, tert-Butyldimethylsilyl chloride 29346-30-3, 3-(Tributylstannyl)-1-propanol 39257-56-2, 2-Iodoethyl cinnamate 52415-29-9, 6-Bromoindole 54060-30-9, 3-Ethynylphenylamine 58313-23-8, Ethyl 3-iodobenzoate 74141-12-1 95037-48-2, 1-Acetylpiperidine-4-carbonyl chloride hydrochloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered

protein tyrosine phosphatase 1B)
IT 9004-10-8, Insulin, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(resistance; preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)
IT **745078-81-3P**, Ethyl 5-[3-[[2-[3-hydroxy-2-(methoxycarbonyl)phenoxy]ethyl]amino]phenyl]isoxazole-3-carboxylate
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of arylazole derivs. as protein-tyrosine phosphatase inhibitors for treating disorders caused by overexpressed or altered protein tyrosine phosphatase 1B)
RN 745078-81-3 HCAPLUS
CN 3-Isoxazolecarboxylic acid, 5-[3-[[2-[3-hydroxy-2-(methoxycarbonyl)phenoxy]ethyl]amino]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)



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L17 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:696360 HCAPLUS
DN 141:225492
ED Entered STN: 26 Aug 2004
TI Preparation of isoxazoles as inhibitors of heat shock proteins
IN Drysdale, Martin James; Dymock, Brian William; Finch, Harry; Webb, Paul; Mcdonald, Edward; James, Karen Elizabeth; Cheung, Kwai Ming; Mathews, Thomas Peter
PA Vernalis Cambridge Limited, UK; Cancer Research Technology Ltd; The Institute of Cancer Research; et al.
SO PCT Int. Appl., 180 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D261-08
ICS C07D413-04; C07D413-10; C07D417-04; C07D261-10; C07D495-04; A61P035-00
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1, 63
FAN.CNT 1

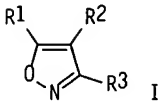
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004072051	A1	20040826	WO 2004-GB506	20040209

W: AE, AE, AG, AL, AL, AM, AM, AM, AT, AT, AU, AZ, AZ, BA, BB, BG, BG, BR, BR, BW, BY, BY, BZ, BZ, CA, CH, CN, CN, CO, CO, CR, CR, CU, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EC, EC, EE, EE, EG, ES, ES, FI, FI, GB, GD, GE, GE, GH, GM, HR, HR, HU, HU, ID, IL, IN, IS, JP, JP, KE, KE, KG, KG, KP, KP, KP, KR, KR, KZ, KZ, KZ, LC, LK, LR, LS, LS, LT, LU, LV, MA, MD, MD, MG, MK, MN, MW, MX, MX,

MZ, MZ, NA, NI
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
PRAI GB 2003-3105 A 20030211
GB 2003-6560 A 20030321
GB 2003-13751 A 20030613
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2004072051	ICM	C07D261-08
	ICS	C07D413-04; C07D413-10; C07D417-04; C07D261-10; C07D495-04; A61P035-00
WO 2004072051	ECLA	C07D261/08; C07D261/10; C07D413/04+319+261; C07D413/10+261+211; C07D413/10+261+213; C07D413/10307B+261; C07D417/04+277B+261; C07D495/04+333B+235B

OS MARPAT 141:225492
GI



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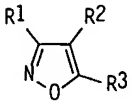

II

AB Title compds. [I, II; R1 = Ar1(Alk1)p(Z)r(Alk2)sQ; Ar1 = (substituted) aryl, heteroaryl; Alk1, Alk2 = (substituted) alkylene, alkenylene; p, r, s = 0, 1; Z = O, S, CO, CS, SO2, CO2, CONRA, CSNRA, SO2NRA, NRACO, NRASO2, NRA; RA = H, alkyl; Q = H, (substituted) carbocyclyl, heterocyclyl; R2 = Ar1(Alk1)p(Z)r(Alk2)sQ, carboxamide, carbocyclyl, heterocyclyl optionally substituted by (Alk1)pZr(Alk2)sQ; R3 = H, (substituted) cycloalkyl, cycloalkenyl, alkyl, alkenyl, alkynyl, carboxyl, carboxamide, carboxyl ester], were prepared Thus, NH2OH.HCl and 7-hydroxy-3-(4-methoxyphenyl)-2-methylchromen-4-one (preparation given) were refluxed 4 h in pyridine to give 4-[4-(4-methoxyphenyl)-3-methylisoxazol-5-yl]benzene-1,3-diol. The latter in the Malachite Green ATPase assay inhibited HSP90 with IC50 <50 .mu.M.
ST isoxazole prepn heat shock protein inhibitor; cancer viral infection arthritis asthma multiple sclerosis treatment arylisoxazole
IT Brain, disease
Prion diseases
(Creutzfeldt-Jakob, treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Heat-shock proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(HSP 70; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Heat-shock proteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(HSP 90, inhibitors; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Nervous system, disease
(Huntington's chorea, treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Eye, disease
(diabetic retinopathy, treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Uterus, disease
(endometriosis, treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Apoptosis

(failure treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Blood vessel, neoplasm
(hemangioma, treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Intestine, disease
(inflammatory, treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Diabetes mellitus
(insulin-dependent, treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Anti-Alzheimer's agents
Antiasthmatics
Antidiabetic agents
Antirheumatic agents
Antitumor agents
Antiviral agents
Drug delivery systems
Human
(preparation of isoxazoles as inhibitors of heat shock proteins)
IT Brain, disease
Prion diseases
(scrapie, treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Chemotherapy
(toxicity treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Alzheimer's disease
Asthma
Cystic fibrosis
Hypoxia, animal
Ischemia
Lupus erythematosus
Multiple sclerosis
Neoplasm
Psoriasis
Rheumatoid arthritis
(treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT Infection
(viral, treatment; preparation of isoxazoles as inhibitors of heat shock proteins)
IT 747412-76-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(claimed compound; preparation of isoxazoles as inhibitors of heat shock proteins)
IT 747412-49-3P 747412-50-6P 747412-51-7P 747412-52-8P 747412-53-9P
747412-54-0P 747412-55-1P 747412-56-2P 747412-57-3P 747412-58-4P
747412-59-5P 747412-60-8P 747412-61-9P 747412-62-0P 747412-63-1P
747412-64-2P 747412-65-3P 747412-66-4P **747412-67-5P**
747412-68-6P 747412-69-7P 747412-70-0P
747412-71-1P 747412-72-2P 747412-73-3P 747412-74-4P
747412-75-5P 747412-77-7P 747412-78-8P 747756-97-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of isoxazoles as inhibitors of heat shock proteins)
IT 747413-08-7P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of isoxazoles as inhibitors of heat shock proteins)

IT 303057-32-1P 303057-40-1P 305342-42-1P 305867-28-1P 314243-75-9P
374703-12-5P 380322-08-7P 747412-79-9P 747412-80-2P
747412-83-5P 747412-84-6P 747412-85-7P 747412-86-8P
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747413-79-2P 747413-80-5P **747413-81-6P** **747413-82-7P**
747413-83-8P 747413-85-0P 747413-87-2P **747413-89-4P**
747413-90-7P **747413-91-8P** **747413-92-9P**
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747413-99-6P **747414-00-2P** **747414-01-3P**
747414-02-4P **747414-03-5P** 747414-04-6P 747414-05-7P
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747414-32-0P 747414-33-1P 747414-34-2P 747414-35-3P 747414-36-4P
747414-37-5P 747414-38-6P 747414-39-7P 747414-40-0P 747414-41-1P
747414-42-2P 747414-43-3P 747414-44-4P 747414-45-5P 747414-46-6P
747414-47-7P 747414-54-6P 747414-58-0P 747414-59-1P 747414-60-4P
747414-61-5P 747414-68-2P 747414-75-1P 747414-77-3P 747414-81-9P
747414-82-0P 747757-18-2P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoxazoles as inhibitors of heat shock proteins)

IT 75-04-7, Ethylamine, reactions 75-65-0, 2-Methyl-2-propanol, reactions 77-77-0, Divinyl sulfone 79-22-1, Methyl chloroformate 79-31-2, Isobutyric acid 89-84-9 95-88-5, 4-Chlororesorcinol 95-92-1, Diethyl oxalate 98-80-6, Phenylboronic acid 100-52-7, Benzaldehyde, reactions 103-72-0, Phenyl isothiocyanate 104-01-8, 4-Methoxyphenylacetic acid 108-24-7, Acetic anhydride 108-36-1, 1,3-Dibromobenzene 108-46-3, Resorcinol, reactions 109-01-3, N-Methylpiperazine 110-91-8, Morpholine, reactions 131-56-6, 2,4-Dihydroxybenzophenone 141-78-6, Ethyl acetate, reactions 405-50-5, 4-Fluorophenylacetic acid 541-41-3, Ethyl chloroformate 619-66-9, 4-Formylbenzoic acid 700-87-8, 2-Methoxyphenyl isocyanate 1663-39-4, tert-Butyl acrylate 1765-93-1, 4-Fluorophenylboronic acid 1779-49-3, Methyltriphenylphosphonium bromide 2591-86-8, N-Formylpiperidine 2896-60-8, 4-Ethylresorcinol 3680-02-2, Methyl vinyl sulfone 3964-57-6, Methyl 3-chloro-4-hydroxybenzoate 4068-78-4, Methyl 5-chloro-2-hydroxybenzoate 4755-77-5, Ethyl chlorooxoacetate 5720-07-0, 4-Methoxyphenylboronic acid 6783-05-7, trans-2-Phenylvinylboronic acid 39546-32-2, Isonipecotamide 63503-60-6, 3-Chlorobenzeneboronic acid 66698-28-0, 1-(4-Bromophenyl)piperazine 75705-21-4, 4-Aminomethylphenylboronic acid hydrochloride 87199-16-4, 3-Formylbenzeneboronic acid 364794-79-6 477218-10-3 558643-26-8 747414-83-1 747414-85-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of isoxazoles as inhibitors of heat shock proteins)

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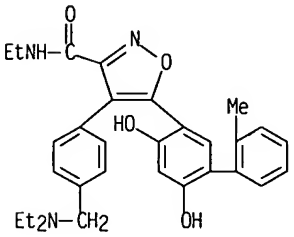
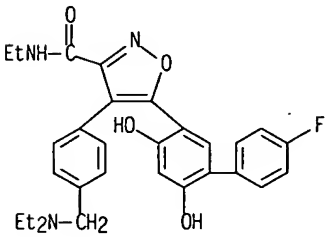
747414-80-8P 747414-84-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoxazoles as inhibitors of heat shock proteins)

IT **747412-67-5P 747412-68-6P 747412-69-7P**
747412-70-0P 747412-71-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(claimed compound; preparation of isoxazoles as inhibitors of heat shock proteins)

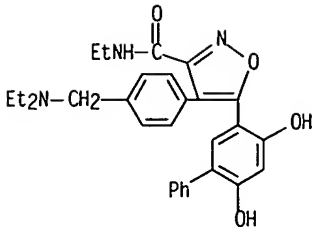
RN 747412-67-5 HCAPLUS
CN 3-Isoxazolecarboxamide, 4-[4-[(diethylamino)methyl]phenyl]-5-(4,6-dihydroxy-2'-methyl[1,1'-biphenyl]-3-yl)-N-ethyl- (9CI) (CA INDEX NAME)



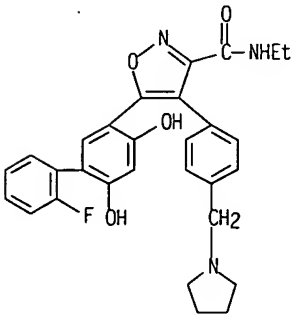
RN 747412-68-6 HCAPLUS
CN 3-Isoxazolecarboxamide, 4-[4-[(diethylamino)methyl]phenyl]-N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)- (9CI) (CA INDEX NAME)



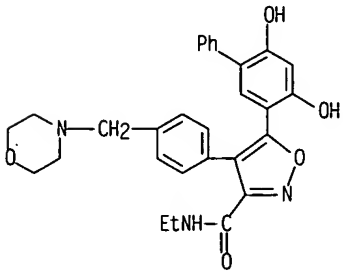
RN 747412-69-7 HCAPLUS
CN 3-Isoxazolecarboxamide, 4-[4-[(diethylamino)methyl]phenyl]-5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl- (9CI) (CA INDEX NAME)



RN 747412-70-0 HCAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(2'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(1-pyrrolidinylmethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 747412-71-1 HCAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-(4-morpholinylmethyl)phenyl]- (9CI) (CA INDEX NAME)



IT **747412-83-5P 747413-77-0P 747413-81-6P**
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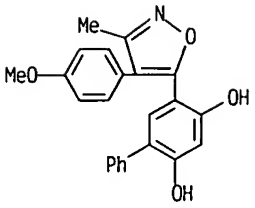
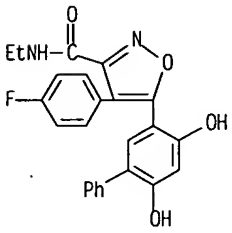
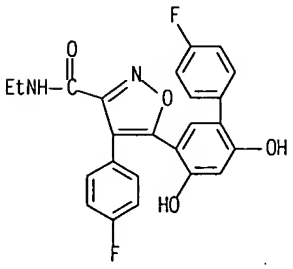
747414-02-4P 747414-03-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of isoxazoles as inhibitors of heat shock proteins)
RN 747412-83-5 HCAPLUS
CN [1,1'-Biphenyl]-2,4-diol, 5-[4-(4-methoxyphenyl)-3-methyl-5-isoxazolyl]- (9CI) (CA INDEX NAME)



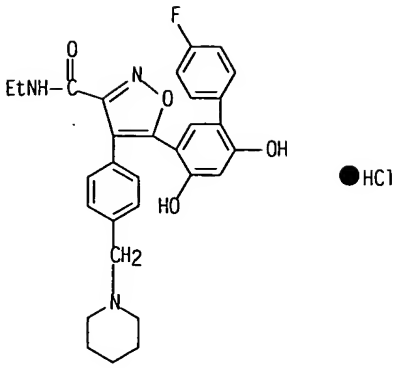
RN 747413-77-0 HCAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl-4-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



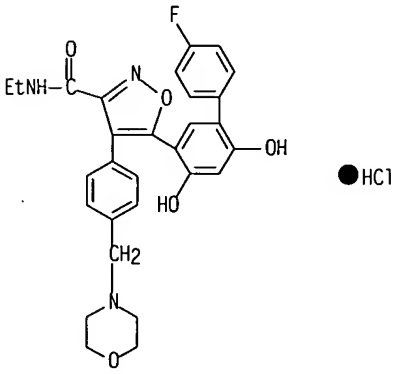
RN 747413-81-6 HCAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-(4-fluorophenyl)- (9CI) (CA INDEX NAME)



RN 747413-82-7 HCAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(1-piperidinylmethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



RN 747413-83-8 HCAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(4-morpholinylmethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



RN 747413-89-4 HCAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-(1-piperidinylmethyl)phenyl]-, monoacetate (salt) (9CI) (CA INDEX NAME)

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CRN 747413-88-3
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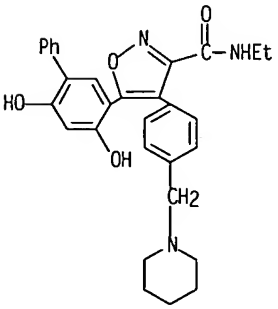

CM 2

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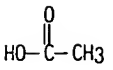
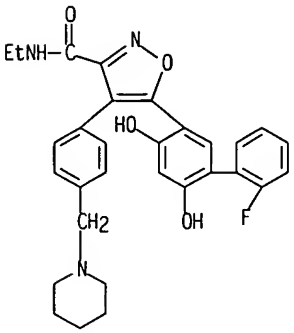
CMF C2 H4 O2

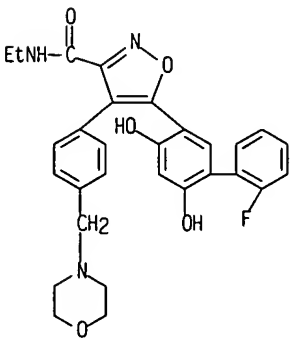


RN 747413-91-8 HCAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(2'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(1-piperidinylmethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)



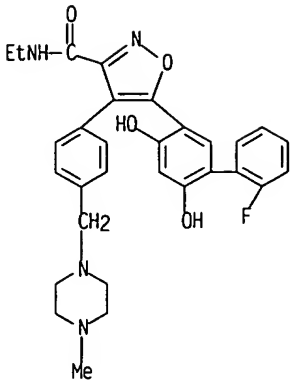
●HCl

RN 747413-92-9 HCAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(2'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-(4-morpholinylmethyl)phenyl]-, monohydrochloride (9CI) (CA INDEX NAME)

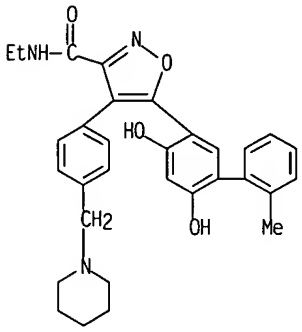


●HCl

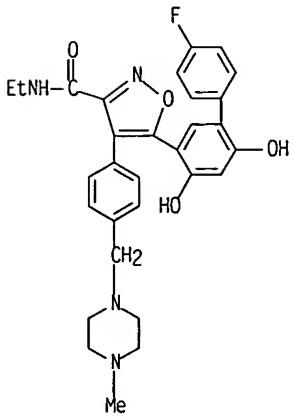
RN 747413-93-0 HCAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(2'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)



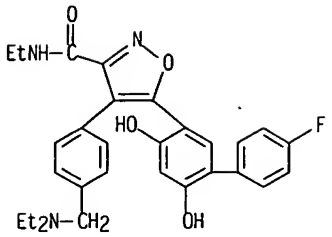
RN 747413-98-5 HCAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy-2'-methyl[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-(1-piperidinylmethyl)phenyl]- (9CI) (CA INDEX NAME)



RN 747414-00-2 HCAPLUS
CN 3-Isoxazolecarboxamide, N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-4-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

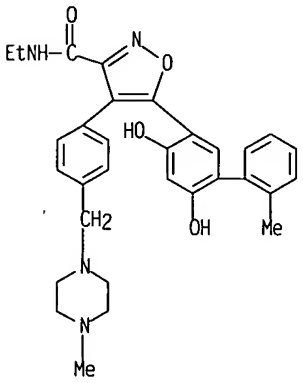


RN 747414-01-3 HCAPLUS
CN 3-Isoxazolecarboxamide, 4-[4-[(diethylamino)methyl]phenyl]-N-ethyl-5-(4'-fluoro-4,6-dihydroxy[1,1'-biphenyl]-3-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

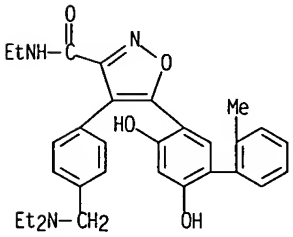


●HCl

RN 747414-02-4 HCAPLUS
CN 3-Isoxazolecarboxamide, 5-(4,6-dihydroxy-2'-methyl[1,1'-biphenyl]-3-yl)-N-ethyl-4-[4-[(4-methyl-1-piperazinyl)methyl]phenyl]- (9CI) (CA INDEX NAME)

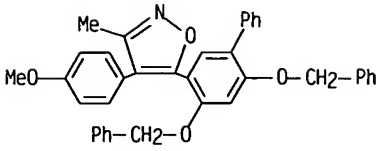


RN 747414-03-5 HCAPLUS
CN 3-Isoxazolecarboxamide, 4-[4-[(diethylamino)methyl]phenyl]-5-(4,6-dihydroxy-2'-methyl[1,1'-biphenyl]-3-yl)-N-ethyl-, monohydrochloride (9CI) (CA INDEX NAME)



●HCl

IT **747412-82-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of isoxazoles as inhibitors of heat shock proteins)
RN 747412-82-4 HCAPLUS
CN Isoxazole, 5-[4,6-bis(phenylmethoxy)[1,1'-biphenyl]-3-yl]-4-(4-methoxyphenyl)-3-methyl- (9CI) (CA INDEX NAME)



L17 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:814125 HCAPLUS
DN 137:325438
ED Entered STN: 25 Oct 2002
TI Preparation of dihydro-benzo[b][1,4]diazepin-2-one derivatives as metabotropic glutamate receptor 2 (mGluR2) antagonists
IN Adam, Geo; Goetschi, Erwin; Mutel, Vincent; Wichmann, Juergen; Woltering, Thomas Johannes
PA F. Hoffmann-La Roche AG, Switz.
SO PCT Int. Appl., 116 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D403-10
ICS A61K031-5513; C07D401-04; C07D403-14; C07D417-10; A61P025-00
CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002083665	A1	20021024	WO 2002-EP3643	20020402
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	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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	EP 1379522	A1	20040114	EP 2002-735209	20020402
	EP 1379522	B1	20050126		
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	NO 2003004496	A	20031008	NO 2003-4496	20031008
PRAI	EP 2001-109126	A	20010412		
	WO 2002-EP3643	W	20020402		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2002083665	ICM	C07D403-10
	ICS	A61K031-5513; C07D401-04; C07D403-14; C07D417-10; A61P025-00
JP 2004525965	FTERM	4C063/AA01; 4C063/BB02; 4C063/CC19; 4C063/CC22; 4C063/CC25; 4C063/CC41; 4C063/CC51; 4C063/CC52; 4C063/CC62; 4C063/DD04; 4C063/DD12; 4C063/DD19; 4C063/EE01; 4C086/AA01; 4C086/AA02; 4C086/AA03; 4C086/AA04; 4C086/BC56; 4C086/BC60; 4C086/BC67; 4C086/BC69; 4C086/BC82; 4C086/GA07; 4C086/GA08;

4C086/GA09; 4C086/GA10; 4C086/MA01; 4C086/MA04;
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4C086/MA66; 4C086/NA14; 4C086/ZA02; 4C086/ZA08;
4C086/ZA11; 4C086/ZA15; 4C086/ZA16; 4C086/ZA18;
4C086/ZA36; 4C086/ZC39; 4C086/ZC42

US 2002198197 ECLA C07D401/04+243+213; C07D403/10+249+243;
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OS MARPAT 137:325438

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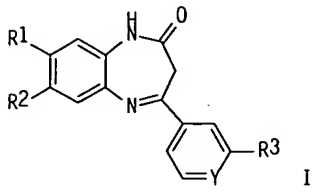


I

AB This invention is concerned with dihydro-benzo[b][1,4]diazepin-2-one derivs. of general formula [I: R1 = cyano, each (un)substituted fluoro-lower alkyl, lower alkoxy, fluoro-lower alkoxy, or is pyrrol-1-yl; R2 = H, if R1 is optionally substituted pyrrol-1-yl as defined above, or R2 = halogen, HO, lower alkyl, fluoro-lower alkyl, lower alkoxy, hydroxymethyl, hydroxyethoxy, lower alkoxy(ethoxy)n (n = 1-4), lower alkoxymethyl, cyanomethoxy, morpholin-4-yl, thiomorpholin-4-yl, 1-oxothiomorpholin-4-yl, 1,1-dioxothiomorpholin-4-yl, 4-oxopiperidin-1-yl 4-alkoxypiperidin-1-yl, 4-hydroxypiperidin-1-yl, 4-hydroxyethoxypiperidin-1-yl, 4-lower alkylpiperazin-1-yl, alkoxycarbonyl, 2-dialkylaminoethylsulfanyl, N,N-bis(lower alkyl)amino-lower alkyl, carbamoylmethyl, etc.; Y = CH, N; R3 = halogen, lower alkyl, fluoro-lower alkyl, lower alkoxy, cyano, -(CH2)nCO-OR''-(CH2)n-CO-NR'R'', or (un)substituted five-membered aromatic heterocycle; R' = H, lower alkyl, C3-6-cycloalkyl, fluoro-lower alkyl or 2-lower alkoxy-lower alkyl; R" = H, lower alkyl, C3-6-cycloalkyl, fluoro-lower alkyl, 2-lower alkoxy lower alkyl, -(CH2)2-4-di-lower alkylamino, -(CH2)2-4-morpholinyl, -(CH2)2-4-pyrrolidinyl, -(CH2)2-4-piperidinyl, 3-hydroxy-lower alkyl; n = 0-4] and their pharmaceutically acceptable addition salts. The invention further relates to medicaments containing these compds. and a process for their preparation as well as their use for preparation of medicaments for the treatment or prevention of acute and/or chronic neurol. disorders including psychosis, schizophrenia, Alzheimer's disease, cognitive disorders and memory deficits. Thus, a mixture of (2-amino-5-thiomorpholin-4-yl-4-trifluoromethylphenyl)carbamic acid tert-Bu ester and 3-(2-cyanopyridin-4-yl)-3-oxopropionic acid tert-Bu ester in toluene was heated to 80-120.degree. to give [2-[3-(2-cyanopyridin-4-yl)-3-oxopropionylamino]-5-thiomorpholin-4-yl-4-trifluoromethylphenyl]carbamic acid tert-Bu ester which was treated with CF3CO2H in CH2Cl2 to give 4-(4-Oxo-8-thiomorpholin-4-yl-7-trifluoromethyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)pyridine-2-carbonitrile (II). II in vitro inhibited the [3H]-LY354740 binding on mGluR2 transfected CHO cell membranes with Ki of 0.0009 .mu.M.

ST dihydrobenzodiazepin prepn metabotropic glutamate receptor 2 antagonist; mGluR2 antagonist dihydrobenzodiazepin prepn; neurol disorder treatment prevention dihydrobenzodiazepin prepn; psychosis schizophrenia Alzheimer disease treatment prevention dihydrobenzodiazepin prepn; cognitive disorder memory deficit treatment prevention dihydrobenzodiazepin prepn

IT Mental disorder
(cognitive; preparation of dihydro-benzo[b][1,4]diazepinone derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment or prevention of acute and/or chronic neurol. disorders)

IT Cognition
(disorder: preparation of dihydro-benzo[b][1,4]diazepinone derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment or prevention of acute and/or chronic neurol. disorders)

IT Glutamate receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(metabotropic, mGluR2: preparation of dihydro-benzo[b][1,4]diazepinone derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment or prevention of acute and/or chronic neurol. disorders)

IT Alzheimer's disease
Anti-Alzheimer's agents
Antipsychotics
Nervous system, disease
Schizophrenia
(preparation of dihydro-benzo[b][1,4]diazepinone derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment or prevention of acute and/or chronic neurol. disorders)

IT Mental disorder
(psychosis; preparation of dihydro-benzo[b][1,4]diazepinone derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment or prevention of acute and/or chronic neurol. disorders)

IT Memory, biological
(retention defect; preparation of dihydro-benzo[b][1,4]diazepinone derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment or prevention of acute and/or chronic neurol. disorders)

IT 473538-96-4P, 3-(4-Oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473538-99-7P, 4-(3-Iodophenyl)-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-11-6P, 2-[3-[4-Oxo-7-pyrrol-1-yl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]phenyl]thiazole-4-carboxylic acid ethyl ester 473539-16-1P, 5-[3-[4-Oxo-7-pyrrol-1-yl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]phenyl]oxazole-4-carboxylic acid ethyl ester 473539-18-3P, 2-[3-(4-Oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)phenyl]oxazole-4-carboxylic acid methyl ester 473539-19-4P, 4-[3-(4-Hydroxymethyloxazol-2-yl)phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-21-8P, 4-[3-[4-Oxo-7-pyrrol-1-yl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]phenyl]thiazole-2-carboxylic acid ethyl ester 473539-41-2P, 4-[3-(5-Hydroxymethyl-[1,2,3]triazol-1-yl)phenyl]-7-methoxy-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-47-8P, 7-Ethoxy-4-[3-(5-hydroxymethyl-[1,2,3]triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-58-1P, 7-Chloro-4-[3-(5-hydroxymethyl-[1,2,3]triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-59-2P, 7-Chloro-4-[3-(5-hydroxymethyl-[1,2,4]triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-63-8P, 4-[3-(5-Hydroxymethyl-[1,2,3]triazol-1-yl)phenyl]-7-methyl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(intermediate; preparation of dihydro-benzo[b][1,4]diazepin-2-one derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment and/or prevention of acute and/or chronic neurol. disorders)

IT 1087-21-4P, Isophthalic acid diallyl ester 46425-21-2P, Isophthalic acid monoallyl ester 53503-61-0P, tert-Butyl lithioacetate 59896-23-0P, 3-Chlorocarbonylbenzoic acid allyl ester 335255-81-7P, 3-Oxo-3-(3-([1,2,3]triazol-1-yl)phenyl)propionic acid ethyl ester 335255-82-8P, 3-[1,2,3]Triazol-1-ylbenzoic acid 335255-83-9P, 3-(3-Cyanophenyl)-3-oxopropionic acid tert-butyl ester 335255-84-0P 335255-85-1P, Methyl 3-(1H-imidazol-1-yl)benzoate 335255-88-4P, 3-Oxo-3-(3-([1,2,4]triazol-1-yl)phenyl)propionic acid tert-butyl ester 335255-95-3P 335256-03-6P, 3-[3-(3-Methylisoxazol-5-yl)phenyl]-3-oxopropionic acid tert-butyl ester 335256-24-1P, 3-(2,2-Dimethyl-6-oxo-

6H-[1,3]dioxin-4-yl)benzonitrile 335256-25-2P 335256-29-6P, 6-(3-Iodophenyl)-2,2-dimethyl-[1,3]dioxin-4-one 335256-30-9P 335256-34-3P, 6-(3-(Imidazol-1-yl)phenyl)-2,2-dimethyl-[1,3]dioxin-4-one 335256-35-4P, 3-(3-Imidazol-1-ylphenyl)-3-oxopropionic acid 335256-44-5P, 4-(2,2-Dimethyl-6-oxo-6H-[1,3]dioxin-4-yl)pyridine-2-carbonitrile 335349-73-0P, (5-Cyanomethyl-4-iodo-2-nitrophenyl)carbamic acid tert-butyl ester 335349-74-1P, (5-Amino-2-iodo-4-nitrophenyl)acetonitrile 428871-73-2P, 5-Fluoro-2-nitro-4-trifluoromethylphenylamine 454464-55-2P, Methyl 3-(2-bromopropionyl)benzoate 473537-10-9P, (5-Fluoro-2-nitro-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-14-3P, (2-Nitro-4-(pyrrol-1-yl)phenyl)carbamic acid tert-butyl ester 473537-16-5P, 2-Nitro-4-(pyrrol-1-yl)phenylamine 473537-18-7P, [5-(2-Methoxyethoxy)-2-nitro-4-(pyrrol-1-yl)phenyl]carbamic acid tert-butyl ester 473537-20-1P, 5-(2-Methoxyethoxy)-2-nitro-4-(pyrrol-1-yl)phenylamine 473537-22-3P, (5-Methoxy-2-nitro-4-(pyrrol-1-yl)phenyl)carbamic acid tert-butyl ester 473537-24-5P, 5-Methoxy-2-nitro-4-(pyrrol-1-yl)phenylamine 473537-26-7P, [4-(2-tert-Butylpyrrol-1-yl)-5-methoxy-2-nitrophenyl]carbamic acid tert-butyl ester 473537-31-4P, (5-Methoxy-2-nitro-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-32-5P, 5-Methoxy-2-nitro-4-trifluoromethylphenylamine 473537-34-7P, (5-Ethoxy-2-nitro-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-36-9P, 5-Ethoxy-2-nitro-4-trifluoromethylphenylamine 473537-38-1P, (4-Cyano-5-fluoro-2-nitrophenyl)carbamic acid tert-butyl ester 473537-41-6P, (5-Chloro-2-nitro-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-43-8P, (5-(Morpholin-4-yl)-2-nitro-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-45-0P 473537-47-2P, (4-Cyano-5-(morpholin-4-yl)-2-nitrophenyl)carbamic acid tert-butyl ester 473537-48-3P 473537-49-4P, (5-Methyl-2-nitro-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-50-7P, 5-Chloro-2-nitro-4-(pyrrol-1-yl)phenylamine 473537-51-8P, 2-Nitro-5-(pyrrol-1-yl)phenylamine 473537-52-9P, 1-(3-Amino-4-nitrophenyl)-4-(2-chlorophenyl)-1H-pyrrole-3-carbonitrile 473537-53-0P, 1-(3-Amino-4-nitrophenyl)-4-phenyl-1H-pyrrole-3-carbonitrile 473537-55-2P, 4-Iodo-2-nitro-5-(pyrrol-1-yl)phenylamine 473537-56-3P, N-(5-Amino-4-iodo-2-nitrophenyl)acetamide 473537-57-4P, 1-(3-Amino-4-nitrophenyl)-1H-pyrrole-3-carboxaldehyde 473537-58-5P, [1-(3-Amino-4-nitrophenyl)-1H-pyrrol-3-yl]methanol 473537-59-6P, 2-Nitro-5-(3-phenylpyrrol-1-yl)phenylamine 473537-60-9P 473537-61-0P, 2,5-Dimethoxy-3-methoxymethyltetrahydrofuran 473537-62-1P 473537-63-2P, 1-(3-Amino-4-nitrophenyl)-1H-pyrrole-2-carboxylic acid methyl ester 473537-64-3P, (2-Amino-5-(morpholin-4-yl)-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-65-4P, (2-Amino-4-(pyrrol-1-yl)phenyl)carbamic acid tert-butyl ester 473537-66-5P, [2-Amino-5-(2-methoxyethoxy)-4-(pyrrol-1-yl)phenyl]carbamic acid tert-butyl ester 473537-67-6P, (2-Amino-5-methoxy-4-(pyrrol-1-yl)phenyl)carbamic acid tert-butyl ester 473537-68-7P, [2-Amino-4-(2-tert-butylpyrrol-1-yl)-5-methoxyphenyl]carbamic acid tert-butyl ester 473537-69-8P, (2-Amino-5-cyanomethyl-4-iodophenyl)carbamic acid tert-butyl ester 473537-70-1P 473537-71-2P, [2-Amino-5-(1,1-dioxo-thiomorpholin-4-yl)-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473537-72-3P, [5-(1,1-Dioxo-thiomorpholin-4-yl)-2-nitro-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473537-73-4P, (2-Amino-5-methoxy-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-74-5P, (2-Amino-5-fluoro-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-75-6P, (2-Amino-5-ethoxy-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-76-7P, (2-Amino-4-cyano-5-(morpholin-4-yl)phenyl)carbamic acid tert-butyl ester 473537-77-8P 473537-78-9P, (2-Amino-5-chloro-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-79-0P, (2-Amino-5-methyl-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-80-3P 473537-81-4P 473537-82-5P 473537-83-6P, 2-(3-Methylisoxazol-5-yl)isonicotinic acid methyl ester 473537-84-7P

473537-85-8P, 3-(2-Methyl-2H-pyrazol-3-yl)benzoic acid methyl ester 473537-86-9P, 3-[3-(5-Dimethylaminomethyl-[1,2,3]triazol-1-yl)phenyl]-3-oxopropionic acid tert-butyl ester 473537-87-0P, 3-(5-((Dimethylamino)methyl)-[1,2,3]triazol-1-yl)benzoic acid methyl ester 473537-88-1P, 3-[3-(3-Methoxymethylisoxazol-5-yl)phenyl]-3-oxopropionic acid tert-butyl ester 473537-89-2P, Methyl 3-(3-methoxymethylisoxazol-5-yl)benzoate 473537-90-5P 473537-91-6P 473537-93-8P 473537-94-9P 473537-95-0P, (RS)-3-Oxo-3-[3-[5-((tetrahydropyran-2-yloxy)methyl)isoxazol-3-yl]phenyl]propionic acid tert-butyl ester 473537-96-1P, (RS)-3-[5-((Tetrahydropyran-2-yloxy)methyl)isoxazol-3-yl]benzoic acid methyl ester 473537-97-2P, 3-Oxo-3-(3-(pyrazol-1-yl)phenyl)propionic acid tert-butyl ester 473537-98-3P, 3-Oxo-3-(3-([1,2,3]triazol-1-yl)phenyl)propionic acid tert-butyl ester 473537-99-4P 473538-00-0P 473538-01-1P 473538-02-2P 473538-03-3P, 3-Oxo-3-[3-(5-methyloxazol-4-yl)phenyl]propionic acid tert-butyl ester 473538-04-4P, Methyl 3-(5-methyloxazol-4-yl)benzoate 473538-05-5P 473538-06-6P, Methyl 3-(2-hydroxymethyl-5-methylthiazol-4-yl)benzoate 473538-07-7P, Methyl 3-[5-methyl-2-((tetrahydropyran-2-yloxy)methyl)thiazol-4-yl]benzoate 473538-08-8P, 3-Oxo-3-[3-[5-methyl-2-((tetrahydropyran-2-yloxy)methyl)thiazol-4-yl]phenyl]propionic acid tert-butyl ester 473538-09-9P, 3-Oxo-3-[3-[4-((tetrahydropyran-2-yloxy)methyl)thiazol-2-yl]phenyl]propionic acid tert-butyl ester 473538-10-2P, 3-(4-Hydroxymethylthiazol-2-yl)benzoic acid methyl ester 473538-11-3P, 3-[4-((Tetrahydropyran-2-yloxy)methyl)thiazol-2-yl]benzoic acid methyl ester 473538-12-4P, 2,2-Dimethyl-6-(3-oxazol-2-ylphenyl)-[1,3]dioxin-4-one 473538-13-5P, 3-(3-Oxazol-2-ylphenyl)-3-oxopropionic acid 473538-14-6P, 3-(Oxazol-2-yl)benzoyl chloride 473538-15-7P, 3-[N-(2,2-Dimethoxyethyl)aminocarbonyl]benzoic acid methyl ester 473538-16-8P, 3-[N-(2-Oxoethyl)aminocarbonyl]benzoic acid methyl ester 473538-17-9P, 3-(Oxazol-2-yl)benzoic acid methyl ester 473538-18-0P, 3-(Oxazol-2-yl)benzoic acid 473538-20-4P, 5-[3-(2,2-Dimethyl-6-oxo-6H-[1,3]dioxin-4-yl)phenyl]oxazole-4-carboxylic acid ethyl ester 473538-22-6P, 5-(3-Carboxyacetylphenyl)oxazole-4-carboxylic acid ethyl ester 473538-23-7P, 5-(3-Chlorocarbonylphenyl)oxazole-4-carboxylic acid ethyl ester 473538-24-8P, 5-(3-Allyloxycarbonylphenyl)oxazole-4-carboxylic acid ethyl ester 473538-25-9P, 5-(3-Carboxyphenyl)oxazole-4-carboxylic acid ethyl ester 473538-26-0P, 2-[3-(2,2-Dimethyl-6-oxo-6H-[1,3]dioxin-4-yl)phenyl]oxazole-4-carboxylic acid methyl ester 473538-27-1P, 2-(3-Carboxyacetylphenyl)oxazole-4-carboxylic acid methyl ester 473538-28-2P, 2-(3-Chlorocarbonylphenyl)oxazole-4-carboxylic acid methyl ester 473538-29-3P 473538-30-6P, (S)-2-(3-Allyloxycarbonylphenyl)-4,5-dihydrooxazole-4-carboxylic acid methyl ester 473538-31-7P, 2-(3-Allyloxycarbonylphenyl)oxazole-4-carboxylic acid methyl ester 473538-32-8P, 2-(3-Carboxyphenyl)oxazole-4-carboxylic acid methyl ester 473538-33-9P, 4-[3-(2,2-Dimethyl-6-oxo-6H-[1,3]dioxin-4-yl)phenyl]thiazole-2-carboxylic acid ethyl ester 473538-34-0P, 4-(3-Carboxyacetylphenyl)thiazole-2-carboxylic acid ethyl ester 473538-35-1P, 4-(3-Chlorocarbonylphenyl)thiazole-2-carboxylic acid ethyl ester 473538-36-2P, 4-(3-Carboxyphenyl)thiazole-2-carboxylic acid ethyl ester 473538-37-3P 473538-38-4P 473538-39-5P, [2-[[3-(2-Cyano-pyridin-4-yl)-3-oxopropionyl]amino]-5-(morpholin-4-yl)-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473538-40-8P**, [2-[[3-[3-(3-Methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-morpholin-4-yl-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-41-9P 473538-42-0P, [2-[[3-(3-Cyanophenyl)-3-oxopropionyl]amino]-4-(pyrrol-1-yl)phenyl]carbamic acid tert-butyl ester 473538-43-1P, N-[5-[3-(2-Chlorophenyl)-4-cyano-pyrrol-1-yl]-2-nitrophenyl]-3-(3-cyanophenyl)-3-oxopropionamide 473538-44-2P, 3-(3-Cyanophenyl)-N-[5-(3-cyano-4-phenylpyrrol-1-yl)-2-nitrophenyl]-3-oxopropionamide 473538-45-3P, 3-(3-Iodophenyl)-N-(2-nitro-4-(pyrrol-1-yl)phenyl)-3-oxopropionamide 473538-46-4P, 3-(3-Cyanophenyl)-N-(4-iodo-2-nitro-5-(pyrrol-1-yl)phenyl)-3-oxopropionamide 473538-47-5P, [2-[[3-(3-Cyanophenyl)-3-oxopropionyl]amino]-5-(2-methoxyethoxy)-4-(pyrrol-1-yl)phenyl]carbamic acid tert-butyl ester 473538-48-6P,

3-(3-Cyanophenyl)-N-[5-(3-hydroxymethylpyrrol-1-yl)-2-nitrophenyl]-3-oxopropionamide 473538-49-7P, 3-(3-Cyanophenyl)-N-[2-nitro-5-(3-phenylpyrrol-1-yl)phenyl]-3-oxopropionamide 473538-50-0P, 3-(3-Cyanophenyl)-N-[5-(3-methoxymethylpyrrol-1-yl)-2-nitrophenyl]-3-oxopropionamide 473538-51-1P, 3-(3-Cyanophenyl)-N-[5-(2-methoxymethylpyrrol-1-yl)-2-nitrophenyl]-3-oxopropionamide 473538-52-2P, 1-[3-[[3-(3-Cyanophenyl)-3-oxopropionyl]amino]-4-nitrophenyl]-1H-pyrrole-2-carboxylic acid methyl ester 473538-53-3P, 3-(3-(Imidazol-1-yl)phenyl)-N-(2-nitro-5-(pyrrol-1-yl)phenyl)-3-oxopropionamide 473538-54-4P, [2-[[3-(3-(Imidazol-1-yl)phenyl)-3-oxopropionyl]amino]-4-(pyrrol-1-yl)phenyl]carbamic acid tert-butyl ester 473538-55-5P, [2-[[3-(3-Cyanophenyl)-3-oxopropionyl]amino]-5-methoxy-4-(pyrrol-1-yl)phenyl]carbamic acid tert-butyl ester 473538-56-6P, [4-(2-tert-Butylpyrrol-1-yl)-2-[[3-(3-cyanophenyl)-3-oxopropionyl]amino]-5-methoxyphenyl]carbamic acid tert-butyl ester 473538-57-7P, [2-[[3-Oxo-3-(3-([1,2,3]triazol-1-yl)phenyl)propionyl]amino]-4-(pyrrol-1-yl)phenyl]carbamic acid tert-butyl ester 473538-58-8P, [5-Cyanomethyl-2-[[3-(3-(imidazol-1-yl)phenyl)-3-oxopropionyl]amino]-4-iodophenyl]carbamic acid tert-butyl ester 473538-59-9P, [2-[[3-[3-(2-Methyl-2H-pyrazol-3-yl)phenyl]-3-oxopropionyl]amino]-5-(morpholin-4-yl)-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473538-60-2P** 473538-61-3P, [2-[[3-[3-(5-((Dimethylamino)methyl)-[1,2,3]triazol-1-yl)phenyl]-3-oxopropionyl]amino]-5-(morpholin-4-yl)-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473538-62-4P**, [2-[[3-[3-(3-Methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-thiomorpholin-4-yl-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-63-5P, [2-[[3-(2-Cyano-pyridin-4-yl)-3-oxopropionyl]amino]-5-thiomorpholin-4-yl-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-64-6P 473538-65-7P, [2-[[3-(2-Cyano-pyridin-4-yl)-3-oxopropionyl]amino]-5-methoxy-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473538-66-8P**, [5-Methoxy-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-67-9P 473538-68-0P 473538-69-1P, [5-(Morpholin-4-yl)-2-[[3-oxo-3-(3-(pyrazol-1-yl)phenyl)propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-70-4P, [5-(Morpholin-4-yl)-2-[[3-oxo-3-(3-(4H-[1,2,4]triazol-4-yl)phenyl)propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-71-5P 473538-72-6P 473538-73-7P, [2-[[3-(2-Cyano-pyridin-4-yl)-3-oxopropionyl]amino]-5-ethoxy-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-74-8P, [5-Ethoxy-2-[[3-oxo-3-(3-([1,2,3]triazol-1-yl)phenyl)propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-75-9P, [5-Methoxy-2-[[3-oxo-3-(3-([1,2,3]triazol-1-yl)phenyl)propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-76-0P, [2-[[3-(2-Cyano-pyridin-4-yl)-3-oxopropionyl]amino]-5-methyl-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-77-1P, [5-Cyano-2-[[3-(3-cyanophenyl)-3-oxopropionyl]amino]-4-(morpholin-4-yl)phenyl]carbamic acid tert-butyl ester 473538-78-2P **473538-79-3P**, [4-Cyano-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(morpholin-4-yl)phenyl]carbamic acid tert-butyl ester 473538-80-6P **473538-81-7P**, [5-Chloro-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-83-9P **473538-84-0P**, [5-Methyl-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-85-1P, [5-Chloro-2-[[3-oxo-3-(3-([1,2,4]triazol-1-yl)phenyl)propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-86-2P, [5-Chloro-2-[[3-(3-(imidazol-1-yl)phenyl)-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-87-3P, [5-Chloro-2-[[3-oxo-3-(3-([1,2,3]triazol-1-yl)phenyl)propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-88-4P, [5-Methyl-2-[[3-oxo-3-(3-([1,2,4]triazol-1-yl)phenyl)propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-89-5P, [5-Methyl-2-[[3-(3-(imidazol-1-yl)phenyl)-

3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-90-8P, [5-Methyl-2-[[3-oxo-3-(3-([1,2,3]triazol-1-yl)phenyl)propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-91-9P, [5-Methyl-2-[[3-oxo-3-(3-(pyrazol-1-yl)phenyl)propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473538-92-0P 473539-12-7P, 3-[4-Oxo-7-pyrrol-1-yl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]thiobenzamide 473539-22-9P, 5-[3-(2,2-Dimethyl-6-oxo-6H-[1,3]dioxin-4-yl)phenyl]thiazole-2-carboxylic acid ethyl ester 473539-30-9P, 4-[3-[4-(Chloromethyl)thiazol-2-yl]phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-74-1P, 4-[3-(4-Chloromethyloxazol-2-yl)phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of dihydro-benzo[b][1,4]diazepin-2-one derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment and/or prevention of acute and/or chronic neurol. disorders)

IT 473538-93-1P, 4-[3-(5-Hydroxymethyl-[1,2,3]triazol-1-yl)phenyl]-7-morpholin-4-yl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473538-94-2P, 4-(8-(Morpholin-4-yl)-4-oxo-7-trifluoromethyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)pyridine-2-carbonitrile 473538-95-3P, 4-[3-(3-Methylisoxazol-5-yl)phenyl]-7-morpholin-4-yl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473538-97-5P, 4-(2-Chlorophenyl)-1-[2-(3-cyanophenyl)-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-7-yl]-1H-pyrrole-3-carbonitrile 473538-98-6P, 1-[2-(3-Cyanophenyl)-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-7-yl]-4-phenyl-1H-pyrrole-3-carbonitrile 473539-00-3P, 3-(4-Oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzamide 473539-01-4P, 3-(8-Iodo-4-oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473539-02-5P, 3-(8-(2-Methoxyethoxy)-4-oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473539-03-6P, 3-(7-(3-Hydroxymethylpyrrol-1-yl)-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473539-04-7P, 3-(4-Oxo-7-(3-phenylpyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473539-05-8P, 3-(7-(3-Methoxymethylpyrrol-1-yl)-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473539-06-9P, 3-[7-(2-Methoxymethylpyrrol-1-yl)-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]benzonitrile 473539-07-0P, 1-[2-(3-Cyanophenyl)-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-7-yl]-1H-pyrrole-2-carboxylic acid methyl ester 473539-08-1P, 4-(3-(Imidazol-1-yl)phenyl)-8-(pyrrol-1-yl)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-09-2P, 3-(8-Methoxy-4-oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473539-10-5P, 3-(7-(2-tert-Butylpyrrol-1-yl)-8-methoxy-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473539-13-8P, 4-[3-(4-Hydroxymethylthiazol-2-yl)phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-14-9P, 8-(Pyrrol-1-yl)-4-(3-([1,2,3]triazol-1-yl)phenyl)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-15-0P, 4-(3-(Oxazol-2-yl)phenyl)-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-17-2P, 5-[3-(4-Oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)phenyl]oxazole-4-carboxylic acid-N-(2-hydroxyethyl)amide 473539-20-7P, 2-[3-(4-Oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)phenyl]oxazole-4-carboxylic acid amide 473539-23-0P, 4-[3-(3-Methylisoxazol-5-yl)phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-24-1P, 4-[3-(4-Oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)phenyl]thiazole-2-carboxylic acid amide 473539-25-2P, 2-[3-[4-Oxo-7-pyrrol-1-yl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]phenyl]oxazole-4-carboxylic acid bis(2-hydroxyethyl)amide 473539-26-3P, 4-[3-(4-Oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)phenyl]thiazole-2-carboxylic acid N-(2-hydroxyethyl)amide 473539-27-4P, 4-[3-(2-Hydroxymethylthiazol-4-yl)phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-28-5P, 2-[3-(4-Oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-

benzo[b][1,4]diazepin-2-yl)phenyl]oxazole-4-carboxylic acid N-(2-hydroxyethyl)amide 473539-29-6P, 4-[3-[4-((Dimethylamino)methyl)thiazol-2-yl]phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-31-0P, 4-[3-(4-Morpholin-4-ylmethylthiazol-2-yl)phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-32-1P, [4-(3-(Imidazol-1-yl)phenyl)-8-iodo-2-oxo-2,3-dihydro-1H-benzo[b][1,4]diazepin-7-yl]acetonitrile 473539-33-2P, 4-[3-(2-Methyl-2H-pyrazol-3-yl)phenyl]-7-morpholin-4-yl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-34-3P, 4-[3-(3-Hydroxymethylisoxazol-5-yl)phenyl]-7-morpholin-4-yl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-35-4P, 4-[3-(5-((Dimethylamino)methyl)-[1,2,3]triazol-1-yl)phenyl]-7-morpholin-4-yl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-36-5P, 4-[3-(3-Methylisoxazol-5-yl)phenyl]-7-thiomorpholin-4-yl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-37-6P 473539-38-7P, 7-(1,1-Dioxo-thiomorpholin-4-yl)-4-[3-(5-hydroxymethyl-[1,2,3]triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-39-8P, 4-(8-Methoxy-4-oxo-7-trifluoromethyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)pyridine-2-carbonitrile 473539-40-1P, 7-Methoxy-4-[3-(3-methylisoxazol-5-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-42-3P, 7-Methoxy-4-[3-[5-pyrrolidin-1-ylmethyl-[1,2,3]triazol-1-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-43-4P, 4-[3-(5-Hydroxymethylisoxazol-3-yl)phenyl]-7-morpholin-4-yl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-44-5P, 7-(Morpholin-4-yl)-4-(3-(pyrazol-1-yl)phenyl)-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-45-6P, 7-(Morpholin-4-yl)-4-(3-(4H-1,2,4-triazol-4-yl)phenyl)-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-46-7P, 7-Fluoro-4-[3-[5-hydroxymethyl-[1,2,3]triazol-1-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-48-9P, 4-[8-Ethoxy-4-oxo-7-trifluoromethyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]pyridine-2-carbonitrile 473539-49-0P, 4-[3-(5-((Cyclopropylamino)methyl)-[1,2,3]triazol-1-yl)phenyl]-7-ethoxy-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-50-3P, 7-Ethoxy-4-[3-(5-[(2,2,2-trifluoroethylamino)methyl]-[1,2,3]triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-51-4P, 7-Ethoxy-4-(3-([1,2,3]triazol-1-yl)phenyl)-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-52-5P 473539-53-6P, 4-(8-Methyl-4-oxo-7-trifluoromethyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)pyridine-2-carbonitrile 473539-54-7P, 2-(3-Cyanophenyl)-8-morpholin-4-yl-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473539-55-8P, 2-[3-(5-Hydroxymethyl-[1,2,3]triazol-1-yl)phenyl]-8-morpholin-4-yl-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473539-56-9P, 2-[3-(3-Methylisoxazol-5-yl)phenyl]-8-morpholin-4-yl-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473539-57-0P, 2-[3-(3-Methylisoxazol-5-yl)phenyl]-4-oxo-8-thiomorpholin-4-yl-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473539-60-5P, 7-Chloro-4-[3-(3-methylisoxazol-5-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-61-6P, 7-Chloro-4-[3-(5-((cyclopropylamino)methyl)-[1,2,4]triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-62-7P, 7-Chloro-4-[3-(5-((cyclopropylamino)methyl)-[1,2,3]triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-64-9P, 4-[3-(5-((Cyclopropylamino)methyl)-[1,2,3]triazol-1-yl)phenyl]-7-methyl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-65-0P, 7-Methyl-4-[3-(3-methylisoxazol-5-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-66-1P, 7-Chloro-4-(3-([1,2,4]triazol-1-yl)phenyl)-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-67-2P, 7-Chloro-4-(3-(imidazol-1-yl)phenyl)-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-68-3P, 7-Chloro-4-(3-([1,2,3]triazol-1-yl)phenyl)-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-69-4P, 7-Methyl-4-(3-([1,2,4]triazol-1-yl)phenyl)-8-trifluoromethyl-1,3-

dihydrobenzo[b][1,4]diazepin-2-one 473539-70-7P, 4-(3-(Imidazol-1-yl)phenyl)-7-methyl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-71-8P, 7-Methyl-4-(3-([1,2,3]triazol-1-yl)phenyl)-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-72-9P, 7-Methyl-4-(3-(pyrazol-1-yl)phenyl)-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-73-0P 473539-75-2P, 4-[3-(4-((Methylamino)methyl)oxazol-2-yl)phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-76-3P, 4-[3-(4-((Dimethylamino)methyl)oxazol-2-yl)phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-77-4P, 4-[3-(4-Morpholin-4-ylmethyloxazol-2-yl)phenyl]-8-pyrrol-1-yl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-78-5P, 4-(4-Oxo-7-(pyrrol-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)pyridine-2-carbonitrile 473539-79-6P, 7-Methyl-4-[3-(5-methyloxazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-80-9P, 4-[3-(2-Hydroxymethyl-5-methylthiazol-4-yl)phenyl]-7-methyl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473539-81-0P, 4-[3-(4-Hydroxymethylthiazol-2-yl)phenyl]-7-methyl-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of dihydro-benzo[b][1,4]diazepin-2-one derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment and/or prevention of acute and/or chronic neurol. disorders)

IT 473537-54-1P, N-(5-Amino-2-nitrophenyl)acetamide
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of dihydro-benzo[b][1,4]diazepin-2-one derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment and/or prevention of acute and/or chronic neurol. disorders)

IT 50-00-0, Formaldehyde, reactions 60-34-4, Methylhydrazine 67-56-1, Methanol, reactions 70-23-5, Ethyl bromopyruvate 74-89-5, Methylamine, reactions 75-12-7, Formamide, reactions 105-56-6, Ethyl cyanoacetate 106-95-6, Allyl bromide, reactions 107-29-9, Acetaldoxime 108-59-8, Dimethyl malonate 109-86-4, 2-Methoxyethanol 109-97-7, Pyrrole 110-87-2, 3,4-Dihydro-2H-pyran 110-91-8, Morpholine, reactions 111-42-2, 2-(2-Hydroxyethylamino)ethanol, reactions 121-91-5, Isophthalic acid, reactions 123-75-1, Pyrrolidine, reactions 123-90-0, Thiomorpholine 124-40-3, Dimethylamine, reactions 127-08-2, Potassium acetate 141-43-5, 2-Aminoethanol, reactions 534-07-6, 1,3-Dichloro-2-propanone 540-88-5, tert-Butyl acetate 696-59-3, 2,5-Dimethoxytetrahydrofuran 753-90-2, 2,2,2-Trifluoroethylamine 765-30-0, Cyclopropylamine 1066-54-2, Trimethylsilylacetylene 1635-61-6, 5-Chloro-2-nitrophenylamine 1711-10-0, 3-Iodobenzoyl chloride 1711-11-1, 3-Cyanobenzoyl chloride 1877-71-0, Isophthalic acid monomethyl ester 2999-46-4, Isocyanoacetic acid ethyl ester 5131-58-8 5307-14-2, 2-Nitro-1,4-phenylenediamine 5470-11-1, Hydroxylamine hydrochloride 5680-80-8, L-Serine methyl ester hydrochloride 6089-04-9 6148-64-7, Ethyl malonate potassium salt 7664-41-7, Ammonia, reactions 13531-48-1, Methyl 3-cyanobenzoate 14798-03-9, Ammonium, reactions 16982-21-1, Ethyl thiooxamate 18457-04-0, Bis(trimethylsilyl) malonate 22483-09-6, Aminoacetaldehyde dimethyl acetal 26196-45-2, 5-Chloro-2-nitro-1,4-phenylenediamine 35375-74-7, 5-Chloro-2-nitro-4-trifluoromethylphenylamine 39658-49-6 40167-37-1, 4-Phenylpyrrole-3-carbonitrile 50634-05-4, 2,5-Dimethoxy-3-tetrahydrofuran-carboxaldehyde 58481-14-4, 2-Cyano-isonicotinic acid ethyl ester 62423-73-8, 3-(2-Bromoacetyl)benzoic acid 67018-94-4, (2,5-Dimethoxytetrahydrofuran-3-yl)methanol 69411-68-3, 4-Amino-2-fluorobenzotrifluoride 71494-93-4, 2-Methoxyacetaldoxime 74738-15-1, 4-(o-Chlorophenyl)pyrrole-3-carbonitrile 75486-33-8, Malonic acid mono-tert-butyl ester potassium salt 91187-05-2, (Z)-3-(Hydroxyiminomethyl)benzoic acid methyl ester 93066-93-4, Methyl 3-azidobenzoate 98560-90-8, 2,5-Dimethoxy-2-methoxymethyltetrahydrofuran 106748-27-0, 3-Thiocarbamoylbenzoic acid

methyl ester 108035-47-8, 3-(1H-Imidazol-1-yl)benzoic acid 115006-21-8, Methyl 3-propionylbenzoate 134579-47-8, 2-Iodoisonicotinic acid methyl ester 135294-85-8 143151-03-5, 4-Cyano-5-fluoro-2-nitroaniline 163852-04-8, 1-(3-Bromophenyl)-3-dimethylaminopropenone 167626-27-9, Methyl 3-(1H-[1,2,4]triazol-1-yl)benzoate 168618-35-7, 3-Pyrazol-1-ylbenzoic acid methyl ester 175204-79-2, 2-(tert-Butylcarbonyloxy)thioacetamide 178742-95-5, Ethyl 3-ethynylbenzoate 207119-66-2, 2,5-Dimethoxy-3-phenyltetrahydrofuran 335256-04-7, Ethyl 3-(3-methylisoxazol-5-yl)benzoate 335256-36-5, 3-(1H-Imidazol-1-yl)benzoyl chloride hydrochloride 335351-27-4, 3-Oxo-3-(3-(4H-[1,2,4]triazol-4-yl)phenyl)propionic acid ethyl ester 473537-92-7, 4-(3-Bromophenyl)-2,4-dioxobutyric acid ethyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of dihydro-benzo[b][1,4]diazepin-2-one derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment and/or prevention of acute and/or chronic neurol. disorders)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Hoffmann La Roche; WO 0129011 A 2001 HCAPLUS

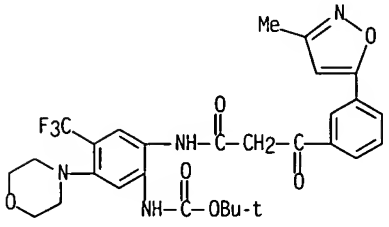
(2) Hoffmann La Roche; WO 0129012 A 2001 HCAPLUS

(3) Pajouhesh, H; WO 0110846 A 2001 HCAPLUS

IT **473538-40-8P**, [2-[[3-[3-(3-Methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-morpholin-4-yl-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473538-60-2P** **473538-62-4P**, [2-[[3-[3-(3-Methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-thiomorpholin-4-yl-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473538-66-8P**, [5-Methoxy-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473538-79-3P**, [4-Cyano-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(morpholin-4-yl)phenyl]carbamic acid tert-butyl ester **473538-81-7P**, [5-Chloro-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473538-84-0P**, [5-Methyl-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of dihydro-benzo[b][1,4]diazepin-2-one derivs. as metabotropic glutamate receptor 2 (mGluR2) antagonists for treatment and/or prevention of acute and/or chronic neurol. disorders)

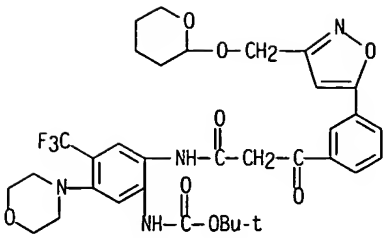
RN 473538-40-8 HCAPLUS

CN Carbamic acid, [2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-(4-morpholinyl)-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

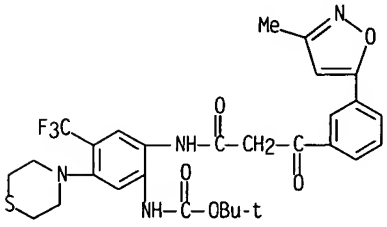


RN 473538-60-2 HCAPLUS

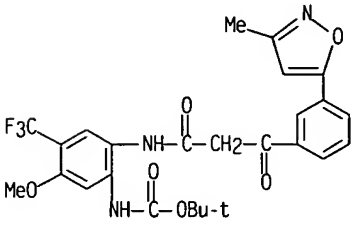
CN Carbamic acid, [2-[[1,3-dioxo-3-[3-[3-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-isoxazolyl]phenyl]propyl]amino]-5-(4-morpholinyl)-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



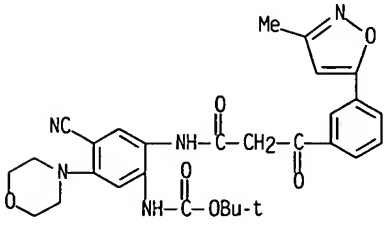
RN 473538-62-4 HCAPLUS
CN Carbamic acid, [2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-(4-thiomorpholinyl)-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 473538-66-8 HCAPLUS
CN Carbamic acid, [5-methoxy-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 473538-79-3 HCAPLUS
CN Carbamic acid, [4-cyano-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-(4-morpholinyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 473538-81-7 HCAPLUS
CN Carbamic acid, [5-chloro-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

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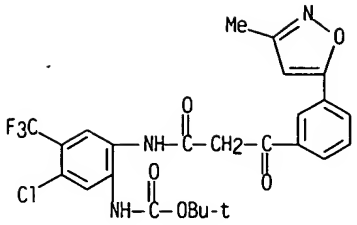

RN 473538-84-0 HCAPLUS
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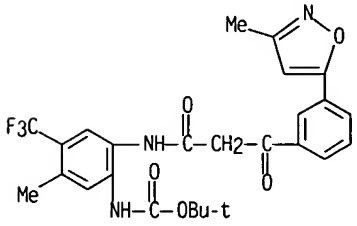

L17 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:814112 HCAPLUS
DN 137:325447
ED Entered STN: 25 Oct 2002
TI Preparation of dihydrobenzo[b][1,4]diazepin-2-ones as mGluR2 antagonists for treatment of neurological disorders
IN Adam, Geo; Goetschi, Erwin; Mutel, Vincent; Wichmann, Juergen; Woltering, Thomas Johannes
PA F. Hoffmann-La Roche AG, Switz.
SO PCT Int. Appl., 202 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D243-12
ICS A61K031-5513; C07D403-10; C07D401-04; C07D403-14; C07D417-10; A61P025-00
CC 28-22 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2002083652	A1	20021024	WO 2002-EP3644	20020402
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CA 2442557	AA	20021024	CA 2002-2442557	20020402
EP 1379511	A1	20040114	EP 2002-737911	20020402
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	BR 2002008891	A	20040420	BR 2002-8891	20020402
	JP 2004529925	T2	20040930	JP 2002-581408	20020402
	US 2002193367	A1	20021219	US 2002-115826	20020403
	US 6544985	B2	20030408		
	NO 2003004576	A	20031112	NO 2003-4576	20031010
	BG 108254	A	20040930	BG 2003-108254	20031010
PRAI	EP 2001-109125	A	20010412		
	WO 2002-EP3644	W	20020402		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2002083652	ICM	C07D243-12
	ICS	A61K031-5513; C07D403-10; C07D401-04; C07D403-14; C07D417-10; A61P025-00
JP 2004529925	FTERM	4C063/AA01; 4C063/AA03; 4C063/BB01; 4C063/BB06; 4C063/CC41; 4C063/CC42; 4C063/CC51; 4C063/CC52; 4C063/CC58; 4C063/CC62; 4C063/CC67; 4C063/DD12; 4C063/DD22; 4C063/DD25; 4C063/DD37; 4C063/EE01; 4C086/AA01; 4C086/AA02; 4C086/AA03; 4C086/AA04; 4C086/BC56; 4C086/BC60; 4C086/BC67; 4C086/BC69; 4C086/BC71; 4C086/BC82; 4C086/BC85; 4C086/MA01; 4C086/MA04; 4C086/NA14; 4C086/ZA02; 4C086/ZA16; 4C086/ZA18; 4C086/ZC42
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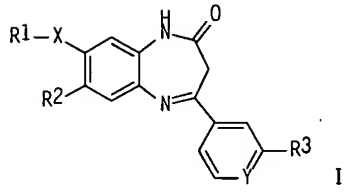
OS MARPAT 137:325447

GI



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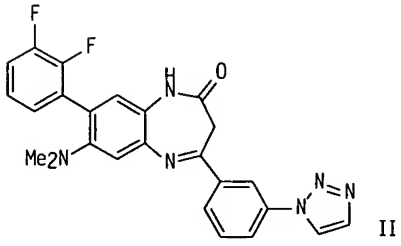

II

AB Title compds. I [wherein X = single bond or ethynediyl group; when X = single bond, R1 = CN , halo, (cyclo)alkyl, (fluoro)alkoxy, fluoroalkyl, or (un)substituted pyrrolyl or Ph; when X = ethynediyl, R1 = (un)substituted Ph; R2 = NR4R5, alkoxy, or R5-(un)substituted oxopiperazinyl, pyrrolidinyl, or piperidinyl; R3 = halo, (fluoro)alkyl, alkoxy, CN, (CH2)nCO2R5, (CH2)nCONR4R5, or (un)substituted 5-membered heteroaryl; R4 = H, (cyclo)alkyl, fluoroalkyl, or alkoxyalkyl; R5 = H, (cyclo)alkyl, fluoroalkyl, alkoxyalkyl, (CH2)m-dialkylamino, (CH2)m-morpholinyl, (CH2)m-pyrrolidinyl, (CH2)m-piperidinyl, or hydroxyalkyl; Y = CH, or N; m = 2-4; n = 0-4; or their pharmaceutically acceptable salts thereof] were prepared as metabotropic glutamate receptor 2 (mGluR2) antagonists. For example, coupling (5-amino-2-dimethylamino-2',3'-difluorobiphenyl-4-

yl)carbamic acid tert-Bu ester with 3-oxo-3-(3-[1,2,3]triazol-1-ylphenyl)propionic acid Et ester (preparation of starting materials given) in toluene afforded the amide, which was cyclized using TFA to give the benzodiazepinone II (Ki = 0.070 .mu.M). Twenty-nine compds. of the invention displayed mGluR2 antagonist activity with Ki values ranging from 0.003 .mu.M to 0.48 .mu.M. Thus, I are useful for the treatment or prevention of acute and/or chronic neurol. disorders, such as psychosis, schizophrenia, Alzheimer's disease, cognitive disorders, and memory deficits (no data).

ST benzodiazepinone prepn mGluR2 antagonist neurol disorder treatment

IT Mental disorder
(cognitive; preparation of benzodiazepinones as mGluR2 antagonists for treatment of neurol. disorders)

IT Cognition
Memory, biological
(disorder; preparation of benzodiazepinones as mGluR2 antagonists for treatment of neurol. disorders)

IT Glutamate receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(metabotropic, mGluR2; preparation of benzodiazepinones as mGluR2 antagonists for treatment of neurol. disorders)

IT Alzheimer's disease
Anti-Alzheimer's agents
Antipsychotics
Cognition enhancers
Human
Nervous system, disease
Nervous system agents
Schizophrenia
(preparation of benzodiazepinones as mGluR2 antagonists for treatment of neurol. disorders)

IT Mental disorder
(psychosis; preparation of benzodiazepinones as mGluR2 antagonists for treatment of neurol. disorders)

IT 115006-21-8P, 3-Propionylbenzoic acid methyl ester 335255-81-7P, 3-Oxo-3-[3-(1,2,3-triazol-1-yl)phenyl]propionic acid ethyl ester 335255-83-9P, 3-(3-Cyanophenyl)-3-oxopropionic acid tert-butyl ester 335255-84-0P 335255-88-4P, 3-Oxo-3-[3-(1,2,4-triazol-1-yl)phenyl]propionic acid tert-butyl ester 335255-95-3P, 3-(2-Cyano-pyridin-4-yl)-3-oxopropionic acid tert-butyl ester 335256-03-6P, 3-[3-(3-Methylisoxazol-5-yl)phenyl]-3-oxopropionic acid tert-butyl ester 335256-24-1P, 3-(2,2-Dimethyl-6-oxo-6H-[1,3]dioxin-4-yl)benzonitrile 335256-25-2P 335256-44-5P, 4-(2,2-Dimethyl-6-oxo-6H-[1,3]dioxin-4-yl)pyridine-2-carbonitrile 335349-57-0P, 5-Chloro-4-iodo-2-nitrophenylamine 335349-60-5P, (5-Chloro-4-iodo-2-nitrophenyl)carbamic acid tert-butyl ester 335350-55-5P 454464-55-2P, 3-(2-Bromopropionyl)benzoic acid methyl ester 473537-10-9P, (5-Fluoro-2-nitro-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-38-1P, (4-Cyano-5-fluoro-2-nitrophenyl)carbamic acid tert-butyl ester 473537-41-6P, (5-Chloro-2-nitro-4-trifluoromethylphenyl)carbamic acid tert-butyl ester 473537-80-3P, 3-Oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]-propionic acid tert-butyl ester 473537-81-4P, 3-[5-(Tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]benzoic acid methyl ester 473537-82-5P, 3-[2-(3-Methylisoxazol-5-yl)pyridin-4-yl]-3-oxopropionic acid tert-butyl ester 473537-84-7P, 3-[3-(2-Methyl-2H-pyrazol-3-yl)phenyl]-3-oxopropionic acid tert-butyl ester 473537-86-9P 473537-88-1P 473537-90-5P, 3-Oxo-3-[3-[3-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]propionic acid tert-butyl ester 473537-91-6P, 3-[3-(Tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]benzoic acid methyl ester 473537-93-8P 473537-94-9P 473537-95-0P, 3-Oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)isoxazol-3-yl]phenyl]propionic acid tert-butyl ester 473537-97-2P, 3-Oxo-3-[3-(pyrazol-1-yl)phenyl]propionic acid tert-butyl ester 473537-98-3P, 3-Oxo-3-[3-(1,2,3-triazol-1-yl)phenyl]propionic acid

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ester 473548-12-8P, 1-[3-(Methoxycarbonyl)phenyl]-1H-pyrazole-4-
carboxylic acid benzyl ester 473548-13-9P, 1-[3-(Methoxycarbonyl)phenyl]-
1H-pyrazole-4-carboxylic acid 473548-14-0P, 3-(4-Hydroxymethylpyrazol-1-
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yl]benzoic acid methyl ester 473548-24-2P 473548-25-3P 473548-26-4P
473548-27-5P, 3-[2-[2-(Tetrahydropyran-2-yloxy)ethyl]-2H-pyrazol-3-

yl]benzoic acid 473548-28-6P, 3-Oxo-3-[3-[5-[2-(tetrahydropyran-2-yloxy)ethyl]-1,2,3-triazol-1-yl]phenyl]propionic acid tert-butyl ester 473548-30-0P, 3-Oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)pyrazol-1-yl]phenyl]propionic acid ethyl ester 473548-31-1P, 3-[5-(Tetrahydropyran-2-yloxymethyl)pyrazol-1-yl]benzoic acid 473548-32-2P, 3-(5-Hydroxymethylpyrazol-1-yl)benzoic acid tert-butyl ester 473548-33-3P, 3-(5-Hydroxymethylpyrazol-1-yl)benzoic acid methyl ester 473548-34-4P, 3-[5-(Tetrahydropyran-2-yloxymethyl)pyrazol-1-yl]benzoic acid methyl ester 473548-35-5P, 3-Oxo-3-[3-(2-bromo-1,1-dimethoxyethyl)phenyl]propionic acid tert-butyl ester 473548-36-6P, 3-(2-Bromo-1,1-dimethoxyethyl)benzoic acid methyl ester 473548-37-7P, 3-Oxo-3-[3-(2-methyloxazol-4-yl)phenyl]propionic acid tert-butyl ester 473548-38-8P, 3-(2-Methyloxazol-4-yl)benzoic acid 473548-39-9P, 3-(2-Methyloxazol-4-yl)benzoic acid methyl ester 473548-40-2P, 3-Oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,3,4-thiadiazol-2-yl]phenyl]propionic acid tert-butyl ester 473548-41-3P 473548-44-6P 473548-45-7P, 3-[5-Hydroxymethyl-1,3,4-thiadiazol-2-yl]benzoic acid methyl ester 473548-46-8P, 3-[5-(Tetrahydropyran-2-yloxymethyl)-1,3,4-thiadiazol-2-yl]benzoic acid methyl ester 473548-47-9P, 3-Oxo-3-[3-[5-[2-(tetrahydropyran-2-yloxy)ethyl]-1,3,4-thiadiazol-2-yl]phenyl]propionic acid tert-butyl ester 473548-48-0P, 3-[5-(2-Hydroxyethyl)-1,3,4-thiadiazol-2-yl]benzoic acid methyl ester 473548-49-1P, 3-[5-[2-(Tetrahydropyran-2-yloxy)ethyl]-1,3,4-thiadiazol-2-yl]benzoic acid methyl ester 473548-50-4P, 3-Oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,3,4-oxadiazol-2-yl]phenyl]propionic acid tert-butyl ester 473548-51-5P, 3-[5-(Hydroxymethyl)-1,3,4-oxadiazol-2-yl]benzoic acid methyl ester 473548-52-6P, 3-Oxo-3-[3-[5-[2-(tetrahydropyran-2-yloxy)ethyl]-1,3,4-oxadiazol-2-yl]phenyl]propionic acid tert-butyl ester 473548-53-7P, 3-[5-(2-Hydroxyethyl)-1,3,4-oxadiazol-2-yl]benzoic acid methyl ester 473548-54-8P 473548-55-9P, 3-(Oxazol-4-yl)benzoic acid methyl ester 473548-56-0P, 3-Oxo-3-[3-(thiazol-4-yl)phenyl]propionic acid tert-butyl ester 473548-57-1P, 3-(Thiazol-4-yl)benzoic acid methyl ester 473548-58-2P 473548-59-3P 473548-60-6P 473548-61-7P, 3-(2-Bromopentanoyl)benzoic acid methyl ester 473548-62-8P, 3-(2-Methyl-5-propyloxazol-4-yl)benzoic acid methyl ester 473548-63-9P 473548-64-0P, 3-(5-Methylthiazol-4-yl)benzoic acid methyl ester 473548-65-1P 473548-66-2P, 3-(2,5-Dimethylthiazol-4-yl)benzoic acid methyl ester 473548-67-3P, 3-Oxo-3-[3-[5-propyl-4-(tetrahydropyran-2-yloxymethyl)thiazol-2-yl]phenyl]propionic acid tert-butyl ester 473548-68-4P, 3-[5-Propyl-4-(tetrahydropyran-2-yloxymethyl)thiazol-2-yl]benzoic acid methyl ester 473548-69-5P, 3-Oxo-3-[3-[2-methyl-5-(tetrahydropyran-2-yloxymethyl)thiazol-4-yl]phenyl]propionic acid tert-butyl ester 473548-70-8P, 3-(5-Bromomethyl-2-methylthiazol-4-yl)benzoic acid methyl ester 473548-71-9P, 3-(5-Hydroxymethyl-2-methylthiazol-4-yl)benzoic acid methyl ester 473548-72-0P, 3-[2-Methyl-5-(tetrahydropyran-2-yloxymethyl)thiazol-4-yl]benzoic acid methyl ester 473548-73-1P, 3-Oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)thiazol-4-yl]phenyl]propionic acid tert-butyl ester 473548-74-2P, 3-(5-Bromomethylthiazol-4-yl)benzoic acid methyl ester 473548-75-3P, 3-(5-Hydroxymethylthiazol-4-yl)benzoic acid methyl ester 473548-76-4P, 3-[5-(Tetrahydropyran-2-yloxymethyl)thiazol-4-yl]benzoic acid methyl ester 473548-77-5P 473548-78-6P, 3-Dihydroxyacetylbenzoic acid methyl ester 473548-79-7P 473548-80-0P, 6-[3-(Imidazol-1-yl)phenyl]-2,2-dimethyl[1,3]dioxin-4-one 473548-81-1P, 2,2-Dimethyl-6-[3-(1,2,3-triazol-1-yl)phenyl][1,3]dioxin-4-one 473548-82-2P, [4-Chloro-2-[[3-(3-cyano-phenyl)-3-oxopropionyl]amino]-5-dimethylaminophenyl]carbamic acid tert-butyl ester 473548-83-3P, [4-Chloro-5-dimethylamino-2-[[3-oxo-3-[3-(1,2,3-triazol-1-yl)phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473548-84-4P, [4-Chloro-5-dimethylamino-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473548-85-5P 473548-86-6P **473548-87-7P** . [4-Chloro-5-dimethylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester 473548-90-2P,

[2-Dimethylamino-2',3'-difluoro-5-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]biphenyl-4-yl]carbamic acid tert-butyl ester 473548-92-4P, [2-Dimethylamino-2',3'-difluoro-5-[[3-oxo-3-[3-(1,2,3-triazol-1-yl)phenyl]propionyl]amino]biphenyl-4-yl]carbamic acid tert-butyl ester 473548-94-6P, [5-[3-(3-Cyanophenyl)-3-oxopropionylamino]-2-dimethylamino-2',3'-difluorobiphenyl-4-yl]carbamic acid tert-butyl ester 473548-95-7P, [4-Chloro-5-dimethylamino-2-[[3-[2-(3-methylisoxazol-5-yl)pyridin-4-yl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester **473548-97-9P** 473548-99-1P 473549-01-8P 473549-02-9P 473549-04-1P, [4-Chloro-2-[[3-(2-cyano-pyridin-4-yl)-3-oxopropionyl]amino]-5-dimethylaminophenyl]carbamic acid tert-butyl ester 473549-05-2P, [4-Chloro-5-dimethylamino-2-[[3-[3-(2-methyl-2H-pyrazol-3-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-06-3P, [5-Dimethylamino-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473549-07-4P**, [5-Dimethylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-08-5P **473549-09-6P**, [4-Chloro-5-dimethylamino-2-[[3-[3-(3-methoxymethylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-10-9P, [2-[[3-(2-Cyano-pyridin-4-yl)-3-oxopropionyl]amino]-5-dimethylamino-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-11-0P **473549-12-1P** 473549-13-2P, [2'-Fluoro-5-[[3-oxo-3-[3-(1,2,3-triazol-1-yl)phenyl]propionyl]amino]-2-(2,2,2-trifluoroethoxy)biphenyl-4-yl]carbamic acid tert-butyl ester 473549-14-3P, [2'-Fluoro-5-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]-2-(2,2,2-trifluoroethoxy)biphenyl-4-yl]carbamic acid tert-butyl ester 473549-15-4P 473549-16-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of benzodiazepinone mGluR2 antagonists by coupling benzenediamines with dioxinones or oxopropanoates followed by cyclization)

IT 473549-17-6P, [4-Chloro-5-(diethylamino)-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-18-7P**, [4-Chloro-5-dimethylamino-2-[[3-oxo-3-[3-[3-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-19-8P, [4-Chloro-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester 473549-20-1P, [5-Dimethylamino-2-[[3-[3-(2-methyl-2H-pyrazol-3-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473549-21-2P**, [4-Chloro-5-dimethylamino-2-[[3-[3-[3-methyl-4-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-22-3P 473549-23-4P 473549-24-5P, [4-Chloro-5-dimethylamino-2-[[3-[3-[2-methyl-5-(tetrahydropyran-2-yloxymethyl)-2H-pyrazol-3-yl]phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-25-6P, [2-[[3-(2-Cyano-pyridin-4-yl)-3-oxopropionyl]amino]-5-(pyrrolidin-1-yl)-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-26-7P, [2-[[3-Oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]-5-(pyrrolidin-1-yl)-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-27-8P, [5-Dimethylamino-4-fluoro-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-28-9P **473549-29-0P**, [5-Dimethylamino-4-fluoro-2-[[3-oxo-3-[3-[3-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-30-3P**, [5-Dimethylamino-2-[[3-oxo-3-[3-[3-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-31-4P,

[4-Chloro-5-dimethylamino-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)isoxazol-3-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-32-5P, [4-Chloro-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]-5-(piperidin-1-yl)phenyl]carbamic acid tert-butyl ester 473549-33-6P, [5-Dimethylamino-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)isoxazol-3-yl]phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-34-7P, [4-Chloro-5-dimethylamino-2-[[3-oxo-3-[3-(pyrazol-1-yl)phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-35-8P, [2-[[3-(2-Cyano-pyridin-4-yl)-3-oxopropionyl]amino]-4-fluoro-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester **473549-36-9P**, [4-Fluoro-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester 473549-37-0P, [4-Fluoro-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester 473549-38-1P, [5-(Azetidin-1-yl)-4-chloro-2-[[3-(2-cyano-pyridin-4-yl)-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-39-2P, [2-[[3-Oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)isoxazol-3-yl]phenyl]propionyl]amino]-5-(pyrrolidin-1-yl)-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-40-5P, [5-(Azetidin-1-yl)-2-[[3-(2-cyano-pyridin-4-yl)-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473549-41-6P**, [5-(Azetidin-1-yl)-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-43-8P, [5-(Azetidin-1-yl)-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-44-9P, [5-Dimethylamino-2-[[3-oxo-3-[3-(pyrazol-1-yl)phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-45-0P, [5-Dimethylamino-2-[[3-[3-(imidazol-1-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-46-1P, [4-Chloro-5-dimethylamino-2-[[3-oxo-3-[3-[4-(tetrahydropyran-2-yloxymethyl)pyrazol-1-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-47-2P, [5-Dimethylamino-2-[[3-oxo-3-[3-[4-(tetrahydropyran-2-yloxymethyl)pyrazol-1-yl]phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473549-48-3P**, [5-Dimethylamino-2-[[3-[3-[3-methyl-4-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-49-4P, [5-Dimethylamino-2-[[3-oxo-3-[3-[4-(tetrahydropyran-2-yloxymethyl)isoxazol-3-yl]phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-50-7P, [5-Dimethylamino-2-[[3-[3-(2-methylsulfanylimidazol-1-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-51-8P, [5-Dimethylamino-2-[[3-[3-[2-methyl-4-(tetrahydropyran-2-yloxymethyl)-2H-pyrazol-3-yl]phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-52-9P, [4-Chloro-5-dimethylamino-2-[[3-oxo-3-[3-(1,2,4-triazol-1-yl)phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-53-0P, [5-Dimethylamino-2-[[3-oxo-3-[3-(1,2,4-triazol-1-yl)phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-54-1P, [2-[[3-(3-Cyanophenyl)-3-oxopropionyl]amino]-5-dimethylamino-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-55-2P 473549-56-3P 473549-57-4P, [5-Dimethylamino-2-[[3-oxo-3-[3-[2-[2-(tetrahydropyran-2-yloxy)ethyl]-2H-pyrazol-3-yl]phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-58-5P 473549-59-6P, [2-Dimethylamino-2'-fluoro-5-[[3-oxo-3-[3-(1,2,3-triazol-1-yl)phenyl]propionyl]amino]biphenyl-4-yl]carbamic acid tert-butyl ester 473549-60-9P, [5-Dimethylamino-2-[[3-oxo-3-[3-[5-[2-(tetrahydropyran-2-yloxy)ethyl]-1,2,3-triazol-1-yl]phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-61-0P, [5-Dimethylamino-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)pyrazol-1-yl]phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-62-1P,

[5-Dimethylamino-2-[[3-oxo-3-[3-(1,2,3-triazol-1-yl)phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-63-2P, [2-[[3-(2-Cyano-pyridin-4-yl)-3-oxopropionyl]amino]-5-(2,2,2-trifluoroethoxy)-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473549-64-3P, [2-[[3-(3-Cyanophenyl)-3-oxopropionyl]amino]-4-dimethylamino-5-methylphenyl]carbamic acid tert-butyl ester 473549-65-4P, [5-Dimethylamino-4-methyl-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-66-5P, [5-Cyano-2-[[3-(3-cyanophenyl)-3-oxopropionyl]amino]-4-dimethylaminophenyl]carbamic acid tert-butyl ester 473549-67-6P, [2-[[3-(3-Cyanophenyl)-3-oxopropionyl]amino]-5-methyl-4-(methylpropylamino)phenyl]carbamic acid tert-butyl ester 473549-68-7P 473549-69-8P 473549-70-1P, [4-Cyano-5-dimethylamino-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-71-2P **473549-72-3P**, [4-Methyl-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(methylpropylamino)phenyl]carbamic acid tert-butyl ester **473549-73-4P**, [4-Cyano-5-dimethylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-74-5P 473549-75-6P**, [5-Dimethylamino-4-methyl-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-76-7P **473549-77-8P** 473549-78-9P, [4-Cyano-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester **473549-79-0P**, [4-Cyano-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester 473549-80-3P **473549-81-4P**, [4-Cyano-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(methylpropylamino)phenyl]carbamic acid tert-butyl ester **473549-82-5P**, [4-Cyano-5-diethylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-83-6P** 473549-84-7P **473549-85-8P** 473549-86-9P **473549-87-0P**, [4-Cyano-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(piperidin-1-yl)phenyl]carbamic acid tert-butyl ester **473549-88-1P**, [4-Chloro-5-isobutylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-89-2P, [4-Chloro-5-isobutylamino-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473549-90-5P **473549-91-6P** 473549-92-7P **473549-93-8P** 473549-94-9P **473549-95-0P** 473549-96-1P **473549-97-2P** 473549-98-3P, [4-Methyl-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester **473549-99-4P**, [4-Methyl-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester **473550-00-4P**, [4-Chloro-5-isopropylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester 473550-01-5P, [4-Chloro-5-isopropylamino-2-[[3-oxo-3-[3-[5-(tetrahydropyran-2-yloxymethyl)-1,2,3-triazol-1-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473550-02-6P 473550-03-7P 473550-04-8P 473550-05-9P 473550-06-0P 473550-07-1P 473550-08-2P 473550-09-3P 473550-10-6P 473550-11-7P 473550-12-8P 473550-13-9P, [2-[[3-[3-(Imidazol-1-yl)phenyl]-3-oxopropionyl]amino]-5-isobutylamino-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473550-14-0P, [4-Chloro-2-[[3-[3-(imidazol-1-yl)phenyl]-3-oxopropionyl]amino]-5-isobutylaminophenyl]carbamic acid tert-butyl ester 473550-15-1P, [4-Chloro-5-(isobutylamino)-2-[[3-oxo-3-[3-(1,2,3-triazol-1-yl)phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473550-16-2P, [5-(Isobutylamino)-2-[[3-oxo-3-[3-(1,2,3-triazol-1-yl)phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473550-17-3P, [4-Chloro-5-(isobutylamino)-2-[[3-oxo-3-

[3-(1,2,4-triazol-1-yl)phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester 473550-18-4P, [5-(Isobutylamino)-2-[[3-oxo-3-[3-(1,2,4-triazol-1-yl)phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester 473550-34-4P, 3-[7-Chloro-8-dimethylamino-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]thiobenzamide 473551-90-5P, 8-Chloro-4-[3-[4-(chloromethyl)thiazol-2-yl]phenyl]-7-dimethylamino-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-93-8P, 4-[3-(Bromoacetyl)phenyl]-8-chloro-7-dimethylamino-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-13-5P, 4-[3-(Bromoacetyl)phenyl]-7-dimethylamino-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473553-34-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzodiazepinone mGluR2 antagonists by coupling benzenediamines with dioxinones or oxopropanoates followed by cyclization)

IT 473546-82-6P, 8-Chloro-7-dimethylamino-4-[3-[4-(hydroxymethyl)thiazol-2-yl]phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-85-9P 473546-96-2P, 8-Chloro-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-7-(isobutylmethylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-99-5P, 8-Chloro-4-[3-[5-(hydroxymethyl)-1,2,4-triazol-1-yl]phenyl]-7-(isobutylmethylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-19-5P, 3-(7-Chloro-8-dimethylamino-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473550-21-9P, 8-Chloro-7-dimethylamino-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-32-2P, 7-Dimethylamino-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-57-1P, 7-Dimethylamino-4-[3-(3-hydroxymethylisoxazol-5-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-77-5P, 7-Dimethylamino-4-[3-(4-hydroxymethylpyrazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-85-5P 473551-00-7P, 8-Chloro-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-7-(isopropylmethylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-13-2P 473551-19-8P 473551-21-2P 473551-33-6P 473551-64-3P 473552-18-0P, 7-Dimethylamino-4-[3-(5-hydroxymethylthiazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(mGluR2 antagonist; preparation of benzodiazepinone mGluR2 antagonists by coupling benzenediamines with dioxinones or oxopropanoates followed by cyclization)

IT 473546-78-0P, 3-[8-Dimethylamino-4-oxo-7-phenylethynyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]benzonitrile 473546-79-1P, 8-(2,3-Difluorophenyl)-7-dimethylamino-4-[3-(1,2,3-triazol-1-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-80-4P, 8-Chloro-7-[(2-methoxyethyl)(methyl)amino]-4-[3-(3-methylisoxazol-5-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-81-5P, 8-Chloro-7-dimethylamino-4-[3-(2-methyl-2H-pyrazol-3-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-83-7P, 8-(2-Fluorophenyl)-4-[3-(3-methylisoxazol-5-yl)phenyl]-7-(2,2,2-trifluoroethoxy)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-84-8P, 8-Chloro-7-dimethylamino-4-[3-[4-(hydroxymethyl)oxazol-2-yl]phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-86-0P, 8-Chloro-7-(diethylamino)-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-87-1P, 8-Chloro-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-7-(pyrrolidin-1-yl)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-88-2P 473546-89-3P, 8-Chloro-7-dimethylamino-4-[3-(pyrazol-1-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-90-6P, 7-Dimethylamino-4-[3-(3-morpholin-4-ylmethylisoxazol-5-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473546-91-7P, 7-Dimethylamino-4-[3-(2-methylsulfanylimidazol-1-yl)phenyl]-8-trifluoromethyl-1,3-

dihydrobenzo[b][1,4]diazepin-2-one 473546-92-8P 473546-93-9P 473546-94-0P, 4-[4-Oxo-8-(2,2,2-trifluoroethoxy)-7-trifluoromethyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]pyridine-2-carbonitrile 473546-95-1P 473546-97-3P, 8-Diethylamino-2-[3-(3-methylisoxazol-5-yl)phenyl]-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473546-98-4P, 4-[3-[5-(Azetidin-1-ylmethyl)-1,2,3-triazol-1-yl]phenyl]-8-chloro-7-(methylpropylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473547-00-1P 473547-01-2P 473547-02-3P, 8-Chloro-4-[3-[4-(hydroxymethyl)thiazol-2-yl]phenyl]-7-(isobutylmethylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473547-03-4P, 8-Chloro-7-dimethylamino-4-[3-(2-ethylaminothiazol-4-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473547-04-5P, 7-Dimethylamino-4-[3-[5-(hydroxymethyl)-1,3,4-thiadiazol-2-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473547-05-6P, 7-Dimethylamino-4-[3-(2-methyl-5-propyloxazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473547-06-7P 473550-20-8P, 8-Chloro-7-dimethylamino-4-[3-(1,2,3-triazol-1-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-22-0P, 7-Dimethylamino-8-phenylethynyl-4-[3-(1,2,3-triazol-1-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-23-1P, 8-Chloro-7-dimethylamino-4-[3-(3-methylisoxazol-5-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-24-2P, 8-(2,3-Difluorophenyl)-7-dimethylamino-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-25-3P, 3-[7-(2,3-Difluorophenyl)-8-dimethylamino-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]benzonitrile 473550-26-4P, 8-Chloro-7-dimethylamino-4-[2-(3-methylisoxazol-5-yl)pyridin-4-yl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-27-5P, 8-Chloro-7-[(2-methoxyethyl)(methyl)amino]-4-[2-(3-methylisoxazol-5-yl)pyridin-4-yl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-28-6P, 8-Chloro-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-7-[(2-methoxyethyl)(methyl)amino]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-29-7P, 8-Chloro-7-[(2-methoxyethyl)(methyl)amino]-4-[3-(1,2,3-triazol-1-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-30-0P, 4-[7-Chloro-8-dimethylamino-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]pyridine-2-carbonitrile 473550-33-3P, 7-Dimethylamino-4-[3-(3-methylisoxazol-5-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-35-5P 473550-36-6P, 8-Chloro-7-dimethylamino-4-[3-(3-methoxymethylisoxazol-5-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-37-7P, 4-[8-Dimethylamino-4-oxo-7-trifluoromethyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]pyridine-2-carbonitrile 473550-38-8P, 8-(2-Fluorophenyl)-4-[3-(imidazol-1-yl)phenyl]-7-(2,2,2-trifluoroethoxy)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-41-3P, 8-(2-Fluorophenyl)-4-[3-(1,2,3-triazol-1-yl)phenyl]-7-(2,2,2-trifluoroethoxy)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-42-4P, 8-(2-Fluorophenyl)-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-7-(2,2,2-trifluoroethoxy)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-43-5P 473550-44-6P, 8-Chloro-7-dimethylamino-4-[3-(3-hydroxymethylisoxazol-5-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-45-7P, 7-Dimethylamino-4-[3-(2-methyl-2H-pyrazol-3-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-46-8P 473550-47-9P, 8-Chloro-7-dimethylamino-4-[3-(4-hydroxymethyl-3-methylisoxazol-5-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-48-0P 473550-49-1P 473550-50-4P, 8-Chloro-7-dimethylamino-4-[3-(5-hydroxymethyl-2-methyl-2H-pyrazol-3-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-51-5P, 4-(4-Oxo-8-(pyrrolidin-1-yl)-7-trifluoromethyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)pyridine-2-carbonitrile 473550-52-6P, 4-[3-[5-(Hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-7-(pyrrolidin-1-yl)-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-53-7P, 7-Dimethylamino-8-fluoro-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-54-8P 473550-55-9P, 7-Dimethylamino-8-fluoro-4-[3-(3-hydroxymethylisoxazol-5-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-56-0P, 8-Chloro-7-dimethylamino-4-[3-[5-(pyrrolidin-1-ylmethyl)-1,2,3-triazol-1-yl]phenyl]-

1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-58-2P, 7-Dimethylamino-8-fluoro-4-[3-(3-methylisoxazol-5-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-60-6P, 4-[3-[5-(Azetidin-1-ylmethyl)-1,2,3-triazol-1-yl]phenyl]-8-chloro-7-dimethylamino-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-61-7P, 8-Chloro-7-dimethylamino-4-[3-(5-hydroxymethylisoxazol-3-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-62-8P, 8-Chloro-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-7-(piperidin-1-yl)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-63-9P, 7-Dimethylamino-4-[3-(5-hydroxymethylisoxazol-3-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-64-0P, 7-Dimethylamino-4-[3-[3-(pyrrolidin-1-ylmethyl)isoxazol-5-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-65-1P 473550-66-2P, 4-[7-Fluoro-4-oxo-8-(pyrrolidin-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]pyridine-2-carbonitrile 473550-67-3P, 8-Fluoro-4-[3-(3-methylisoxazol-5-yl)phenyl]-7-(pyrrolidin-1-yl)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-68-4P, 8-Fluoro-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-7-(pyrrolidin-1-yl)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-69-5P, 4-[8-(Azetidin-1-yl)-7-chloro-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]pyridine-2-carbonitrile 473550-70-8P, 4-[3-(5-Hydroxymethylisoxazol-3-yl)phenyl]-7-(pyrrolidin-1-yl)-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-71-9P, 4-[8-(Azetidin-1-yl)-4-oxo-7-trifluoromethyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl]pyridine-2-carbonitrile 473550-72-0P, 7-(Azetidin-1-yl)-4-[3-(3-methylisoxazol-5-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-73-1P, 7-(Azetidin-1-yl)-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-74-2P, 7-Dimethylamino-4-[3-(pyrazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-75-3P, 7-Dimethylamino-4-[3-(imidazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-76-4P, 8-Chloro-7-dimethylamino-4-[3-(4-hydroxymethylpyrazol-1-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-78-6P, 7-Dimethylamino-4-[3-(4-hydroxymethyl-3-methylisoxazol-5-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-79-7P, 7-Dimethylamino-4-[3-(4-hydroxymethylisoxazol-3-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-80-0P, 7-Dimethylamino-4-[3-(4-hydroxymethyl-2-methyl-2H-pyrazol-3-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-81-1P, 8-Chloro-7-dimethylamino-4-[3-(1,2,4-triazol-1-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-82-2P, 7-Dimethylamino-4-[3-(1,2,4-triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-83-3P, 3-(8-Dimethylamino-4-oxo-7-trifluoromethyl-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473550-84-4P, 7-Dimethylamino-4-[3-[5-[(2,2,2-trifluoroethylamino)methyl]-1,2,3-triazol-1-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-86-6P 473550-87-7P 473550-88-8P, 7-Dimethylamino-4-[3-[2-(2-hydroxyethyl)-2H-pyrazol-3-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-89-9P 473550-90-2P, 7-Dimethylamino-8-(2-fluorophenyl)-4-[3-(1,2,3-triazol-1-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-91-3P, 7-Dimethylamino-4-[3-[5-(2-hydroxyethyl)-1,2,3-triazol-1-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-92-4P, 7-Dimethylamino-4-[3-[5-(hydroxymethyl)pyrazol-1-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-93-5P, 7-Dimethylamino-4-[3-(1,2,3-triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-94-6P, 3-(8-Dimethylamino-7-methyl-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)benzonitrile 473550-95-7P, 7-Dimethylamino-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-8-methyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-96-8P, 2-(3-Cyanophenyl)-8-dimethylamino-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473550-97-9P, 4-[3-[5-(Hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-8-methyl-7-(methylpropylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473550-98-0P 473550-99-1P,

8-Dimethylamino-2-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473551-01-8P, 8-Methyl-4-[3-(3-methylisoxazol-5-yl)phenyl]-7-(methylpropylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-02-9P, 8-Dimethylamino-2-[3-(3-methylisoxazol-5-yl)phenyl]-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473551-03-0P 473551-04-1P, 7-Dimethylamino-8-methyl-4-[3-(3-methylisoxazol-5-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-05-2P 473551-06-3P, 2-[3-[5-(Hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-4-oxo-8-(pyrrolidin-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473551-07-4P, 2-[3-(3-Methylisoxazol-5-yl)phenyl]-4-oxo-8-(pyrrolidin-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473551-08-5P 473551-09-6P 473551-10-9P 473551-11-0P 473551-12-1P 473551-14-3P, 2-[3-(3-Methylisoxazol-5-yl)phenyl]-4-oxo-8-(piperidin-1-yl)-4,5-dihydro-3H-benzo[b][1,4]diazepine-7-carbonitrile 473551-15-4P, 8-Chloro-7-isobutylamino-4-[3-(3-methylisoxazol-5-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-16-5P, 8-Chloro-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-7-isobutylamino-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-17-6P 473551-18-7P 473551-20-1P 473551-22-3P 473551-23-4P 473551-24-5P 473551-25-6P, 8-Chloro-4-[3-[5-[(isopropylmethylamino)methyl]-1,2,3-triazol-1-yl]phenyl]-7-(methylpropylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-26-7P 473551-27-8P 473551-28-9P 473551-29-0P 473551-30-3P, 4-[3-[5-(Azetidin-1-ylmethyl)-1,2,3-triazol-1-yl]phenyl]-8-chloro-7-(isopropylmethylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-31-4P, 4-[3-[5-(Azetidin-1-ylmethyl)-1,2,3-triazol-1-yl]phenyl]-8-chloro-7-(isobutylmethylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-32-5P 473551-34-7P, 4-[3-[5-(Hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-8-methyl-7-(pyrrolidin-1-yl)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-35-8P 473551-36-9P, 8-Methyl-4-[3-(3-methylisoxazol-5-yl)phenyl]-7-(pyrrolidin-1-yl)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-37-0P 473551-38-1P 473551-39-2P 473551-40-5P 473551-41-6P 473551-42-7P 473551-43-8P 473551-44-9P 473551-45-0P 473551-46-1P 473551-47-2P 473551-48-3P 473551-49-4P 473551-50-7P, 8-Chloro-4-[3-[5-[(isobutylmethylamino)methyl]-1,2,3-triazol-1-yl]phenyl]-7-(isopropylmethylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-51-8P 473551-52-9P 473551-53-0P 473551-54-1P 473551-55-2P 473551-56-3P 473551-57-4P 473551-58-5P 473551-59-6P 473551-60-9P 473551-62-1P, 8-Chloro-7-isopropylamino-4-[3-(3-methylisoxazol-5-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-63-2P, 8-Chloro-4-[3-[5-(hydroxymethyl)-1,2,3-triazol-1-yl]phenyl]-7-isopropylamino-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-65-4P 473551-66-5P 473551-67-6P 473551-68-7P 473551-69-8P 473551-70-1P 473551-71-2P 473551-72-3P 473551-73-4P 473551-74-5P 473551-75-6P 473551-76-7P, 4-[3-(Imidazol-1-yl)phenyl]-7-isobutylamino-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-77-8P, 8-Chloro-4-[3-(imidazol-1-yl)phenyl]-7-isobutylamino-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-78-9P, 8-Chloro-7-(isobutylamino)-4-[3-(1,2,3-triazol-1-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-79-0P, 7-(Isobutylamino)-4-[3-(1,2,3-triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-80-3P, 8-Chloro-7-(isobutylamino)-4-[3-(1,2,4-triazol-1-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-81-4P, 7-(Isobutylamino)-4-[3-(1,2,4-triazol-1-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-82-5P 473551-83-6P, 8-Chloro-4-[3-[4-(hydroxymethyl)thiazol-2-yl]phenyl]-7-(methylpropylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-84-7P, 8-Chloro-4-[3-[4-(hydroxymethyl)thiazol-2-yl]phenyl]-7-(isopropylmethylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-85-8P 473551-86-9P, 8-Chloro-4-[3-[4-(hydroxymethyl)oxazol-2-yl]phenyl]-7-(methylpropylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-87-0P, 8-Chloro-4-[3-[4-(hydroxymethyl)oxazol-2-yl]phenyl]-7-(isopropylmethylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-88-1P, 8-Chloro-4-[3-[4-(hydroxymethyl)oxazol-2-yl]phenyl]-7-

(isobutylmethylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-89-2P 473551-91-6P, 8-Chloro-7-dimethylamino-4-[3-[4-(morpholin-4-ylmethyl)thiazol-2-yl]phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-92-7P, 8-Chloro-7-dimethylamino-4-[3-(2-hydroxymethylthiazol-4-yl)phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-94-9P, 4-[3-(2-Aminothiazol-4-yl)phenyl]-8-chloro-7-dimethylamino-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-95-0P, N-[4-[3-(7-Chloro-8-dimethylamino-4-oxo-4,5-dihydro-3H-benzo[b][1,4]diazepin-2-yl)phenyl]thiazol-2-yl]guanidine 473551-96-1P, 8-Chloro-7-dimethylamino-4-[3-[2-(pyridin-4-ylamino)thiazol-4-yl]phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-97-2P, 8-Chloro-4-[3-(2-methyloxazol-4-yl)phenyl]-7-(methylpropylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-98-3P, 4-[3-[4-(Hydroxymethyl)thiazol-2-yl]phenyl]-8-methyl-7-(methylpropylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473551-99-4P, 4-[3-[4-(Hydroxymethyl)oxazol-2-yl]phenyl]-8-methyl-7-(methylpropylamino)-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-00-0P, 7-Dimethylamino-4-[3-[4-(hydroxymethyl)thiazol-2-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-01-1P, 7-Dimethylamino-4-[3-[4-(hydroxymethyl)oxazol-2-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-02-2P 473552-03-3P, 7-Dimethylamino-4-[3-[5-(2-hydroxyethyl)-1,3,4-thiadiazol-2-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-04-4P, 7-Dimethylamino-4-[3-[5-(hydroxymethyl)-1,3,4-oxadiazol-2-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-05-5P, 7-Dimethylamino-4-[3-[5-(2-hydroxyethyl)-1,3,4-oxadiazol-2-yl]phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-06-6P, 7-Dimethylamino-4-[3-(oxazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-07-7P, 7-Dimethylamino-4-[3-(thiazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-08-8P, 7-Dimethylamino-4-[3-(2-methyloxazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-09-9P, 7-Dimethylamino-4-[3-(5-methyloxazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-10-2P, 7-Dimethylamino-4-[3-(5-methylthiazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-11-3P, 7-Dimethylamino-4-[3-(2,5-dimethylthiazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-12-4P, 7-Dimethylamino-4-[3-(2-hydroxymethylthiazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-14-6P, 7-Dimethylamino-4-[3-(2-hydroxymethyl-5-methylthiazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-15-7P, 7-Dimethylamino-4-[3-(2-hydroxymethyl-5-propylthiazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-17-9P, 7-Dimethylamino-4-[3-(5-hydroxymethyl-2-methylthiazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-19-1P 473552-20-4P, 7-Dimethylamino-4-[3-(2-isopropyl-1H-imidazol-4-yl)phenyl]-8-trifluoromethyl-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473552-21-5P, 8-Chloro-7-dimethylamino-4-[3-[5-(2-hydroxyethyl)-1,3,4-thiadiazol-2-yl]phenyl]-1,3-dihydrobenzo[b][1,4]diazepin-2-one 473553-35-4P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(mGluR2 antagonist: preparation of benzodiazepinone mGluR2 antagonists by coupling benzenediamines with dioxinones or oxopropanoates followed by cyclization)

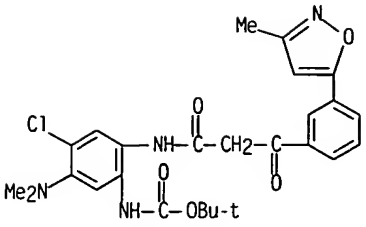
IT 75-31-0, Isopropylamine, reactions 78-67-1, .alpha...alpha.'-Azobis(isobutyronitrile) 78-81-9, Isobutylamine 78-84-2, 2-Methylpropionaldehyde 106-95-6, Allyl bromide, reactions 108-22-5, Isopropenyl acetate 109-84-2, 2-Hydroxyethylhydrazine 109-89-7, N,N-Diethylamine, reactions 110-87-2, Dihydropyran 110-89-4, Piperidine, reactions 110-91-8, Morpholine, reactions 123-75-1, Pyrrolidine, reactions 149-73-5, Trimethyl orthoformate 503-29-7,

Azetidine 534-07-6, 1,3-Dichloro-2-propanone 536-74-3, Phenylacetylene 624-78-2, N-Ethylmethylamine 625-43-4, N-Isobutyl-N-methylamine 625-53-6, N-Ethylthiourea 627-35-0, N-Methylpropylamine 765-30-0, Cyclopropylamine 1003-03-8, Cyclopentylamine 1459-93-4, Dimethyl isophthalate 1635-61-6, 5-Chloro-2-nitroaniline 1711-11-1, 3-Cyanobenzoyl chloride 1993-03-9, 2-Fluorophenylboronic acid 2516-47-4, Cyclopropylmethylamine 4747-21-1, N-Isopropyl-N-methylamine 6148-64-7, Ethyl malonate potassium salt 6641-64-1, 4,5-Dichloro-2-nitroaniline 7149-80-6, 5-Chloro-4-methyl-2-nitroaniline 7252-53-1, Cyclopropylmethylamine hydrochloride 13531-48-1, Methyl 3-cyanobenzoate 18457-04-0, Bis(trimethylsilyl)malonate 20914-88-9, 3-Hydroxypropionimidic acid ethyl ester hydrochloride 26196-45-2, 5-Chloro-2-nitro-1,4-phenylenediamine 32016-27-6, 2-Cyano-3-ethoxyacrylic acid benzyl ester 35375-74-7, 5-Chloro-2-nitro-4-trifluoromethylphenylamine 36743-66-5 36805-97-7 38235-71-1, 3-Hydrazinobenzoic acid 38256-93-8, N-(2-Methoxyethyl)methylamine 53503-61-0, Lithium tert-butyl acetate 58481-14-4, 2-Cyano-isonicotinic acid ethyl ester 62088-13-5 62423-73-8, 3-(2-Bromoacetyl)benzoic acid 67704-17-0, 3-Hydrazinocarbonylbenzoic acid methyl ester 67751-14-8, 4-Dimethylamino-2-oxobut-3-enoic acid ethyl ester 75486-33-8 77335-18-3 81962-58-5, 3-Chloro-4-fluoro-6-nitroacetanilide 93066-93-4, Methyl 3-azidobenzoate 106748-24-7, 3-Carbamoylbenzoic acid methyl ester 106748-27-0, 3-Thiocarbamoylbenzoic acid methyl ester 121219-16-7, 2,3-Difluorophenylboronic acid 135294-85-8, tert-Butyldimethyl[3-(tetrahydropyran-2-yloxy)prop-1-ynyl]silane 143151-03-5, 4-Cyano-5-fluoro-2-nitroaniline 163852-04-8, 1-(3-Bromophenyl)-3-dimethylaminopropenone 164670-44-4, 1-(4-Pyridyl)thiourea 167626-26-8, 3-Hydrazinobenzoic acid methyl ester hydrochloride 168618-35-7, 3-(Pyrazol-1-yl)benzoic acid methyl ester 175204-79-2, 2-(tert-Butylcarbonyloxy)thioacetamide 335255-82-8, 3-(1,2,3-Triazol-1-yl)benzoic acid 335255-85-1, Methyl 3-(1H-imidazol-1-yl)benzoate 335256-01-4 335256-04-7, Ethyl 3-(3-methylisoxazol-5-yl)benzoate 335256-35-4 335351-27-4 428871-73-2, 5-Fluoro-2-nitro-4-trifluoromethylphenylamine 473537-83-6, 2-(3-Methylisoxazol-5-yl)isonicotinic acid methyl ester 473537-85-8, 3-(2-Methyl-2H-pyrazol-3-yl)benzoic acid methyl ester 473537-87-0 473537-89-2, Methyl 3-(3-methoxymethylisoxazol-5-yl)benzoate 473537-92-7 473537-96-1, 3-[5-(Tetrahydropyran-2-yloxymethyl)isoxazol-3-yl]benzoic acid methyl ester 473547-09-0, 4-Iodo-2-nitro-5-(2,2,2-trifluoroethoxy)phenylamine 473547-56-7 473548-02-6, 3-[3-Methyl-4-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]benzoic acid methyl ester 473548-16-2, 3-[4-(Tetrahydropyran-2-yloxymethyl)isoxazol-3-yl]benzoic acid methyl ester 473548-21-9, 3-[2-Methyl-4-(tetrahydropyran-2-yloxymethyl)-2H-pyrazol-3-yl]benzoic acid methyl ester 473548-29-7, 3-[5-[2-(Tetrahydropyran-2-yloxy)ethyl]-1,2,3-triazol-1-yl]benzoic acid methyl ester 473548-42-4 473550-39-9, [2'-Fluoro-5-[[3-[3-(imidazol-1-yl)phenyl]-3-oxopropionyl]amino]-2-(2,2,2-trifluoroethoxy)biphenyl-4-yl]carbamic acid tert-butyl ester **473550-40-2**, [2'-Fluoro-5-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-2-(2,2,2-trifluoroethoxy)biphenyl-4-yl]carbamic acid tert-butyl ester **473550-59-3**, [5-Dimethylamino-4-fluoro-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester 473552-16-8, 3-Oxo-3-[3-[5-propyl-2-(tetrahydropyran-2-yloxymethyl)thiazol-4-yl]phenyl]propionic acid tert-butyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzodiazepinone mGluR2 antagonists by coupling benzenediamines with dioxinones or oxopropanoates followed by cyclization)

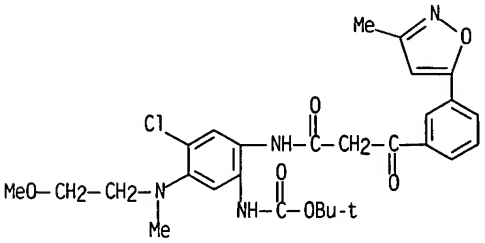
IT 167626-27-9, Methyl 3-(1H-1,2,4-triazol-1-yl)benzoate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of benzodiazepinone mGluR2 antagonists by coupling benzenediamines with dioxinones or oxopropanoates followed by cyclization)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

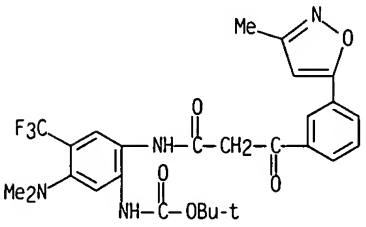
RE
(1) Hoffmann La Roche; WO 0129011 A 2001 HCAPLUS
(2) Hoffmann La Roche; WO 0129012 A 2001 HCAPLUS
(3) Pajouhesh, H; WO 0110846 A 2001 HCAPLUS
IT **473548-87-7P**, [4-Chloro-5-dimethylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester **473548-97-9P 473549-07-4P**, [5-Dimethylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473549-09-6P**, [4-Chloro-5-dimethylamino-2-[[3-[3-(3-methoxymethylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-12-1P 473549-18-7P**, [4-Chloro-5-dimethylamino-2-[[3-oxo-3-[3-[3-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-21-2P**, [4-Chloro-5-dimethylamino-2-[[3-[3-[3-methyl-4-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-29-0P**, [5-Dimethylamino-4-fluoro-2-[[3-oxo-3-[3-[3-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]propionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-30-3P**, [5-Dimethylamino-2-[[3-oxo-3-[3-[3-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]propionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473549-36-9P**, [4-Fluoro-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester **473549-41-6P**, [5-(Azetidin-1-yl)-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473549-48-3P**, [5-Dimethylamino-2-[[3-[3-[3-methyl-4-(tetrahydropyran-2-yloxymethyl)isoxazol-5-yl]phenyl]-3-oxopropionyl]amino]-4-trifluoromethylphenyl]carbamic acid tert-butyl ester **473549-72-3P**, [4-Methyl-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(methylpropylamino)phenyl]carbamic acid tert-butyl ester **473549-73-4P**, [4-Cyano-5-dimethylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-74-5P 473549-75-6P**, [5-Dimethylamino-4-methyl-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-77-8P 473549-79-0P**, [4-Cyano-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester **473549-81-4P**, [4-Cyano-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(methylpropylamino)phenyl]carbamic acid tert-butyl ester **473549-82-5P**, [4-Cyano-5-diethylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-83-6P 473549-85-8P 473549-87-0P**, [4-Cyano-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(piperidin-1-yl)phenyl]carbamic acid tert-butyl ester **473549-88-1P**, [4-Chloro-5-isobutylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester **473549-91-6P 473549-93-8P 473549-95-0P 473549-97-2P 473549-99-4P**, [4-Methyl-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-5-(pyrrolidin-1-yl)phenyl]carbamic acid tert-butyl ester **473550-00-4P**, [4-Chloro-5-isopropylamino-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzodiazepinone mGluR2 antagonists by coupling benzenediamines with dioxinones or oxopropanoates followed by cyclization)
RN 473548-87-7 HCAPLUS
CN Carbamic acid, [4-chloro-5-(dimethylamino)-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



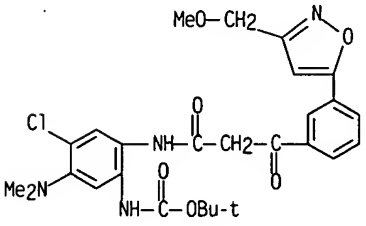
RN 473548-97-9 HCAPLUS
CN Carbamic acid, [4-chloro-5-[(2-methoxyethyl)methylamino]-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 473549-07-4 HCAPLUS
CN Carbamic acid, [5-(dimethylamino)-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

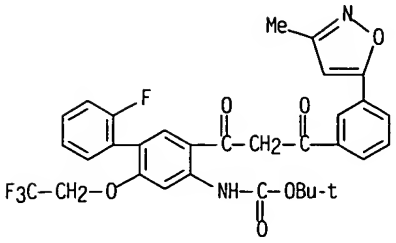


RN 473549-09-6 HCAPLUS
CN Carbamic acid, [4-chloro-5-(dimethylamino)-2-[[3-[3-[3-(methoxymethyl)-5-isoxazolyl]phenyl]-1,3-dioxopropyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

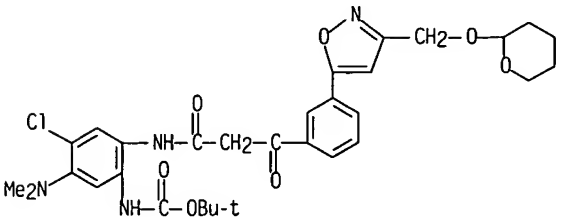


RN 473549-12-1 HCAPLUS
CN Carbamic acid, [2'-fluoro-5-[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]-2-(2,2,2-trifluoroethoxy)[1,1'-biphenyl]-4-yl]-,

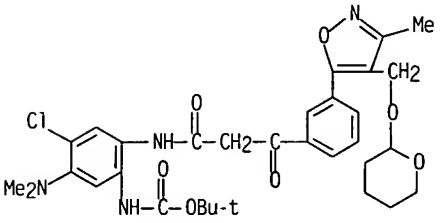
1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



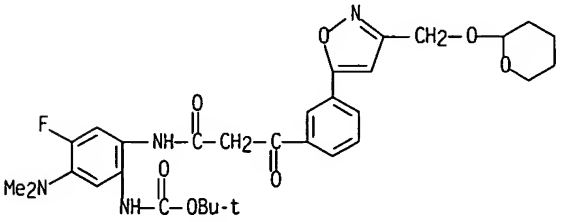
RN 473549-18-7 HCAPLUS
CN Carbamic acid, [4-chloro-5-(dimethylamino)-2-[[1,3-dioxo-3-[3-[3-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-isoxazolyl]phenyl]propyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 473549-21-2 HCAPLUS
CN Carbamic acid, [4-chloro-5-(dimethylamino)-2-[[3-[3-[3-methyl-4-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-isoxazolyl]phenyl]-1,3-dioxopropyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

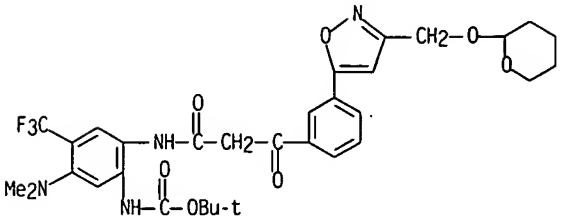


RN 473549-29-0 HCAPLUS
CN Carbamic acid, [5-(dimethylamino)-2-[[1,3-dioxo-3-[3-[3-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-isoxazolyl]phenyl]propyl]amino]-4-fluorophenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

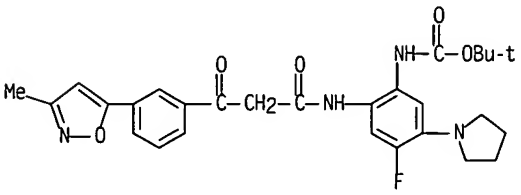


RN 473549-30-3 HCAPLUS
CN Carbamic acid, [5-(dimethylamino)-2-[[1,3-dioxo-3-[3-[3-[[(tetrahydro-2H-

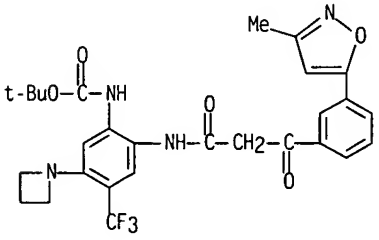
pyran-2-yl)oxy]methyl]-5-isoxazolyl]phenyl]propyl]amino]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



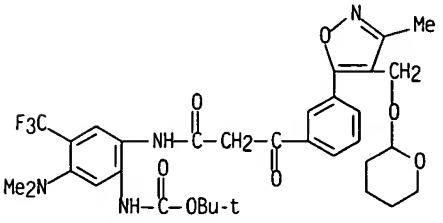
RN 473549-36-9 HCAPLUS
CN Carbamic acid, [4-fluoro-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-(1-pyrrolidinyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 473549-41-6 HCAPLUS
CN Carbamic acid, [5-(1-azetidinyl)-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

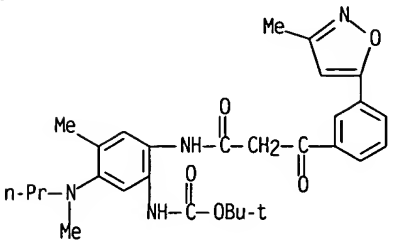


RN 473549-48-3 HCAPLUS
CN Carbamic acid, [5-(dimethylamino)-2-[[3-[3-[3-methyl-4-[[(tetrahydro-2H-pyran-2-yl)oxy]methyl]-5-isoxazolyl]phenyl]-1,3-dioxopropyl]amino]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

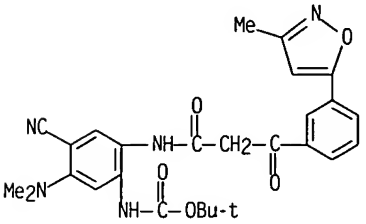


RN 473549-72-3 HCAPLUS
CN Carbamic acid, [4-methyl-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-

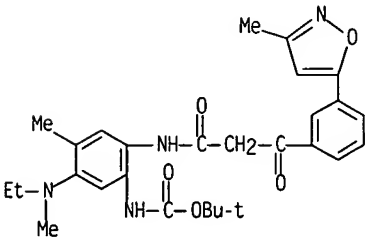
dioxopropyl]amino]-5-(methylpropylamino)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



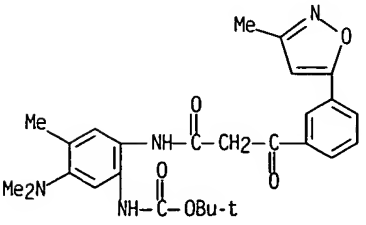
RN 473549-73-4 HCAPLUS
CN Carbamic acid, [4-cyano-5-(dimethylamino)-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



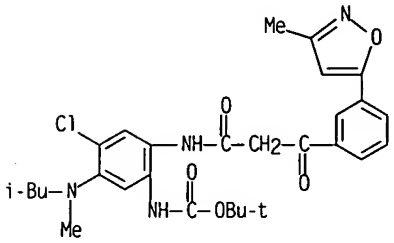
RN 473549-74-5 HCAPLUS
CN Carbamic acid, [5-(ethylmethylamino)-4-methyl-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



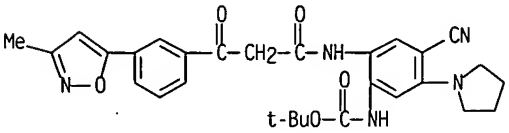
RN 473549-75-6 HCAPLUS
CN Carbamic acid, [5-(dimethylamino)-4-methyl-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



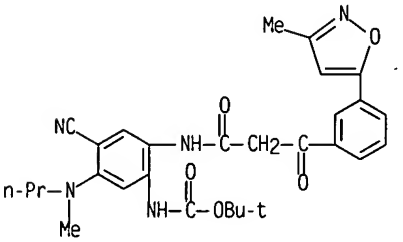
RN 473549-77-8 HCAPLUS
CN Carbamic acid, [4-chloro-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-[methyl(2-methylpropyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



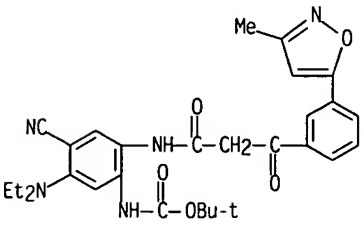
RN 473549-79-0 HCAPLUS
CN Carbamic acid, [4-cyano-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-(1-pyrrolidinyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 473549-81-4 HCAPLUS
CN Carbamic acid, [4-cyano-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-(methylpropylamino)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

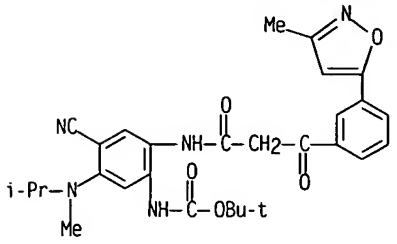


RN 473549-82-5 HCAPLUS
CN Carbamic acid, [4-cyano-5-(diethylamino)-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

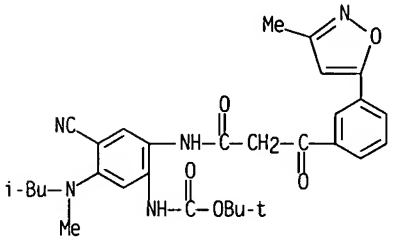


RN 473549-83-6 HCAPLUS

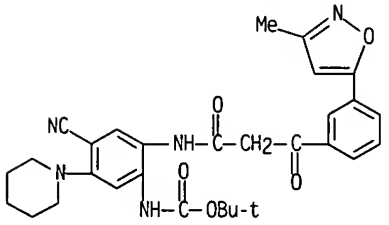
CN Carbamic acid, [4-cyano-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-[methyl(1-methylethyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



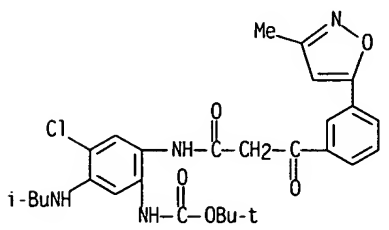
RN 473549-85-8 HCAPLUS
CN Carbamic acid, [4-cyano-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-[methyl(2-methylpropyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



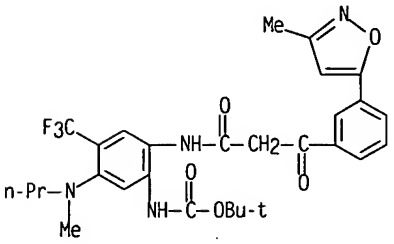
RN 473549-87-0 HCAPLUS
CN Carbamic acid, [4-cyano-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-(1-piperidinyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



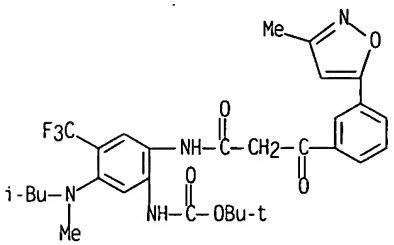
RN 473549-88-1 HCAPLUS
CN Carbamic acid, [4-chloro-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-[(2-methylpropyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



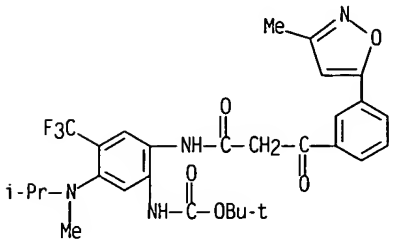
RN 473549-91-6 HCAPLUS
CN Carbamic acid, [2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-(methylpropylamino)-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



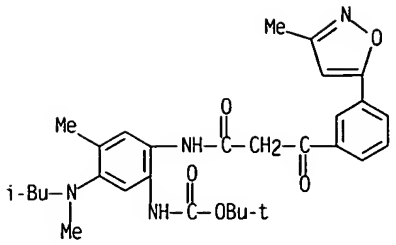
RN 473549-93-8 HCAPLUS
CN Carbamic acid, [2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-[methyl(2-methylpropyl)amino]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



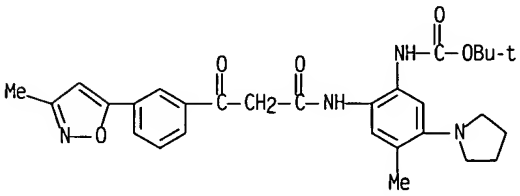
RN 473549-95-0 HCAPLUS
CN Carbamic acid, [2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-[methyl(1-methylethyl)amino]-4-(trifluoromethyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



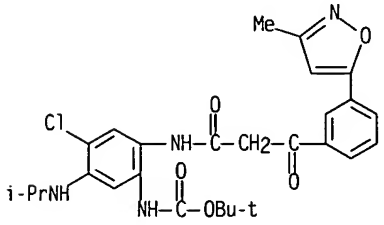
RN 473549-97-2 HCAPLUS
CN Carbamic acid, [4-methyl-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-[methyl(2-methylpropyl)amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 473549-99-4 HCAPLUS
CN Carbamic acid, [4-methyl-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-5-(1-pyrrolidinyl)phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

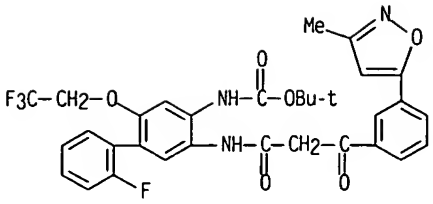


RN 473550-00-4 HCAPLUS
CN Carbamic acid, [4-chloro-5-[(1-methylethyl)amino]-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

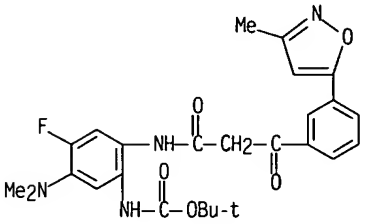


IT **473550-40-2**, [2'-Fluoro-5-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]-2-(2,2,2-trifluoroethoxy)biphenyl-4-yl]carbamic acid tert-butyl ester **473550-59-3**, [5-Dimethylamino-4-fluoro-2-[[3-[3-(3-methylisoxazol-5-yl)phenyl]-3-oxopropionyl]amino]phenyl]carbamic acid tert-butyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzodiazepinone mGluR2 antagonists by coupling benzenediamines with dioxinones or oxopropanoates followed by cyclization)

RN 473550-40-2 HCAPLUS
CN Carbamic acid, [2'-fluoro-5-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]-2-(2,2,2-trifluoroethoxy)[1,1'-biphenyl]-4-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 473550-59-3 HCAPLUS
CN Carbamic acid, [5-(dimethylamino)-4-fluoro-2-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino]phenyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L17 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2002:72091 HCAPLUS
DN 136:134566
ED Entered STN: 25 Jan 2002
TI Synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compounds as .beta.3-adrenergic agonists
IN Evers, Britta; Jesudason, Cynthia Darshini; Karanjawala, Rushad Eruch; Remick, David Michael; Ruehter, Gerd; Sall, Daniel Jon; Schotten, Theo; Siegel, Miles Goodman; Stenzel, Wolfgang; Stucky, Russell Dean; Werner, John Arnold
PA Eli Lilly and Company, USA
SO PCT Int. Appl., 96 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D409-12
ICS C07D401-12; C07D413-12; C07D213-82; C07D405-12; C07D407-12; C07D409-14; C07D417-12; A61K031-44; C07D409-12; C07D333-00; C07D213-00; C07D405-12; C07D303-00; C07D231-00
CC 25-10 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 63
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002006276	A1	20020124	WO 2001-US16519	20010709
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
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	CA 2415331	AA	20020124	CA 2001-2415331	20010709
	AU 2001072917	A5	20020130	AU 2001-72917	20010709

	EP 1303509	A1	20030423	EP 2001-952125	20010709
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	BR 2001012409	A	20030722	BR 2001-12409	20010709
	JP 2004504320	T2	20040212	JP 2002-512179	20010709
	ZA 2002008741	A	20040216	ZA 2002-8741	20021029
	US 2003191156	A1	20031009	US 2002-311112	20021213
	US 6730792	B2	20040504		
	NO 2003000098	A	20030109	NO 2003-98	20030109
	HR 2003000018	A1	20030430	HR 2003-18	20030113
	US 2004242633	A1	20041202	US 2004-838904	20040504
PRAI	US 2000-217965P	P	20000713		
	US 2000-241614P	P	20001019		
	US 2001-292988P	P	20010523		
	WO 2001-US16519	W	20010709		
	US 2002-311112	A1	20021213		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2002006276	ICM	C07D409-12
	ICS	C07D401-12; C07D413-12; C07D213-82; C07D405-12; C07D407-12; C07D409-14; C07D417-12; A61K031-44; C07D409-12; C07D333-00; C07D213-00; C07D405-12; C07D303-00; C07D231-00
JP 2004504320	FTERM	4C023/BA07; 4C033/AA05; 4C033/AA17; 4C033/AA20; 4C033/AD03; 4C033/AD17; 4C033/AD20; 4C037/HA08; 4C037/JA04; 4C048/AA01; 4C048/BB08; 4C048/CC01; 4C055/AA01; 4C055/BA02; 4C055/BA42; 4C055/BB10; 4C055/CA02; 4C055/CA58; 4C055/DA01; 4C056/AA01; 4C056/AB01; 4C056/AC01; 4C056/AC02; 4C056/AD01; 4C056/AE03; 4C056/BA08; 4C056/BC01; 4C056/FA08; 4C063/AA01; 4C063/AA03; 4C063/BB07; 4C063/BB08; 4C063/CC12; 4C063/CC22; 4C063/CC29; 4C063/CC51; 4C063/CC52; 4C063/CC58; 4C063/CC61; 4C063/CC62; 4C063/CC67; 4C063/CC71; 4C063/CC75; 4C063/CC92; 4C063/DD03; 4C063/DD04; 4C063/DD06; 4C063/DD12; 4C063/DD22; 4C063/DD29; 4C063/DD47; 4C063/DD51; 4C063/DD52; 4C063/DD58; 4C063/DD62; 4C063/DD67; 4C063/DD71; 4C063/EE01; 4C063/EE05; 4C086/AA01; 4C086/AA02; 4C086/AA03; 4C086/BA03; 4C086/BB02; 4C086/BC17; 4C086/BC19; 4C086/BC21; 4C086/BC41; 4C086/BC42; 4C086/BC48; 4C086/BC62; 4C086/BC67; 4C086/BC69; 4C086/BC73; 4C086/BC79; 4C086/BC82; 4C086/GA02; 4C086/GA04; 4C086/GA07; 4C086/GA08; 4C086/GA09; 4C086/GA10; 4C086/GA12; 4C086/MA01; 4C086/MA04; 4C086/NA14; 4C086/ZA70; 4C086/ZC35; 4C086/ZC42
US 2003191156	ECLA	C07D207/32C3; C07D213/30C; C07D213/82H; C07D213/84E; C07D261/08; C07D277/24; C07D333/16; C07D401/12+213+209C; C07D401/12+239B+213; C07D401/12+231+213; C07D405/12+307+21; C07D405/12+307B+213; C07D409/12+333+213; C07D409/12+333B+307B; C07D409/12+333B+241B; C07D; C07D413/12+261+241B; C07D413/12+263+213; C07D413/12+261+213; C07D413/12+271+213; C07D417/12+277+241B; C07D417/12+275+213; C07D417/12+277+213; C07D417/12+277+213; C07D417/12+285B+213; C07D417/12+307B+277B
US 2004242633	ECLA	C07D207/32C3; C07D213/30C; C07D213/82H; C07D213/84E; C07D261/08; C07D277/24; C07D333/16; C07D401/12+213+209C; C07D401/12+231+213; C07D401/12+239B+213; C07D405/12+307+21; C07D405/12+307B+213; C07D409/12+333+213; C07D409/12+333B+213; C07D409/12+333B+241B;

C07D409/2+333B+307B; C07D413/12+261+213;
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C07D417/12+277+213; C07D417/12+285B+213;
C07D417/12+307B+277B

OS MARPAT 136:134566

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Title compds. I [A1-3 = C, N provided that only one of A1-3 can be nitrogen; Het = (un)substituted, optionally benzofused 5 or 6 membered heterocyclic ring; R1,1a,1b = H, halo, OH, alkyl, alkoxy, haloalkyl; SO2-alkyl; R2 = H, alkyl; R3 = H alkyl; R4 = H, alkyl; or R3 and R4 combine with the carbon to which both are attached to form a C3-C6 cyclic ring; or R4 and X1 combine with the carbon to which both are attached to form a C3-C8 cyclic ring; or R4 combines with X1, the carbon to which both are attached, and the Ph group to which X1 is attached to form a benzofused cycloalkyl radical; X is OCH2, SCH2, bond; X1 = bond, divalent hydrocarbon moiety; X2 = O, S, NH, NHSO2, SO2NH, CH2, bond; X3 = (un)substituted Ph, 5 or 6 membered heterocyclic ring] were prepared For instance, 2-(1-methylpyrazol-3-yl)phenol was reacted with (2S)-glycidyl 3-nitrobenzenesulfonate (THF, t-BuOK, reflux, 16 h) to give epoxide II. This was reacted with the amine derived from 4-(2-amino-2-methylpropyl)phenol and 2-chloro-3-cyanopyridine (alc. solvent, 80.degree.C, 2-72 h) to give III. The intrinsic activity (Emax) of representative compds. of the invention was assessed relative to isoproterenol (a nonselective .beta.3-agonist); III had Emax = 55.0%. I are used in the treatment of diabetes, obesity, etc.

ST phenol thiophenol beta three adrenergic receptor agonist prepn

IT Lipids, biological studies
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(lipolysis; synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

IT Inflammation
(neurogenic; synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

IT Diabetes mellitus
(non-insulin-dependent; synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

IT Anticholesteremic agents
Antidepressants
Antidiabetic agents
Antiobesity agents
Energy metabolism, animal
Human
Hypolipemic agents
(synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

IT Glycerides, biological studies
Lipoproteins
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

IT Adrenoceptor agonists
(.beta.3-; synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

IT 7683-59-2, Isoproterenol
RL: PAC (Pharmacological activity); BIOL (Biological study)
(comparison; synthesis and use of heteroaryl-substituted-

aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

IT 391920-32-4P 391924-77-9P 391924-79-1P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(drug; synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug; synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug; synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

IT 50-01-1, Guanidine hydrochloride 121-71-1 135-02-4, 2-Methoxybenzaldehyde 611-20-1, 2-Cyanophenol 1452-94-4, Ethyl 2-chloronicotinate 1692-15-5 1776-08-5 2160-62-5, 5-Bromothiophene-2-carbonitrile 2369-37-1, 3,4-Dibromofluorobenzene 4637-24-5 5106-98-9, 4-Chloro-2-hydroxybenzoic acid 5720-06-9, 2-Methoxybenzene boronic acid 6165-68-0 6165-69-1, Thiophene-3-boronic acid 6602-54-6, 2-Chloro-3-cyanopyridine 7417-18-7 13331-23-2 14034-59-4 19438-10-9, Methyl 3-hydroxybenzoate 24065-33-6, 2-Chloro-5-carboxythiophene 32750-21-3, 2-Fluoro-6-iodoanisole 34810-67-8, 2-(Pyrazol-5-yl)phenol 36635-61-7, Tosylmethylisocyanide 51706-55-9 53595-65-6 73781-91-6, Methyl 6-chloronicotinate 87059-79-8 98437-23-1, (Benzothiophen-2-yl)boronic acid 98437-24-2 115314-14-2 123532-22-9, 2-(1-Methylpyrazol-5-yl)phenol 131534-65-1 134598-00-8 150255-96-2, 3-Cyanophenylboronic acid 162607-18-3 162607-20-7 189119-36-6 189119-37-7 189119-38-8 189119-39-9 204592-23-4 204592-30-3 204592-32-5 206551-43-1 340784-31-8 391926-25-3 391926-26-4 391926-27-5 391926-29-7 391926-30-0 391926-31-1 391926-32-2 391926-33-3 391926-34-4 391926-35-5 391926-36-6 391926-37-7 391926-38-8 391926-39-9 391926-40-2

391926-41-3 391926-43-5 391926-44-6 391926-45-7 391926-46-8
391926-48-0 391926-49-1 391926-50-4 391926-51-5 391926-52-6
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391926-58-2 391926-59-3 391926-60-6 391926-61-7 391926-62-8
391926-63-9 391926-64-0 391926-65-1 391926-66-2 391926-67-3
391926-68-4 391926-69-5 391926-70-8 391926-75-3 391926-77-5
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391928-03-3 391928-04-4 391928-05-5 391928-06-6 391928-07-7
391928-08-8 391928-09-9
RL: RCT (Reactant): RACT (Reactant or reagent)
(synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

IT 22353-82-8P, 2-Chloro-5-(carboxamido)thiophene 28177-50-6P 31964-89-3P
33567-59-8P, (2-Methoxyphenyl)acetaldehyde 50478-16-5P,
2-Chloro-5-cyanothiophene 51449-77-5P 65103-28-8P 86723-62-8P
123532-18-3P, 2-(1-Methylpyrazol-3-yl)phenol 340784-59-0P 341510-25-6P
391926-23-1P 391926-24-2P 391926-28-6P 391926-42-4P 391926-47-9P
391926-71-9P 391926-72-0P 391926-73-1P 391926-74-2P 391926-76-4P
391926-87-7P 391926-88-8P 391926-96-8P 391926-97-9P 391926-98-0P
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391927-04-1P 391927-05-2P 391927-07-4P, 4-(2-Benzyloxyphenyl)oxazole
391927-10-9P 391927-23-4P, 2-(5-Cyanothien-2-yl)anisole 391927-27-8P
391927-38-1P 391927-44-9P 391927-45-0P 391927-83-6P 391927-86-9P
391927-90-5P 391927-95-0P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT (Reactant or reagent)
(synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

RE.CNT 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Beecham Group Plc; EP 0236624 A 1987 HCAPLUS
(2) Crowell, T; US 5808080 A 1998 HCAPLUS
(3) Droste, C; WO 9710825 A 1997 HCAPLUS
(4) Droste, C; US 5977154 A 1999 HCAPLUS
(5) Feng, D; WO 9746556 A 1997 HCAPLUS
(6) Mathvink, R; WO 9832753 A 1998 HCAPLUS
(7) Merck & Co Inc; EP 0611003 A 1994 HCAPLUS
(8) Merck & Co Inc; WO 9529159 A 1995 HCAPLUS
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(10) Sankyo Co; EP 0678511 A 1995 HCAPLUS
(11) Shuker, A; TETRAHEDRON LETTERS 1997, V38(35), P6149 HCAPLUS
(12) Tanabe Seiyaku Co; FR 2447904 A 1980 HCAPLUS
(13) Weber, A; BIOORGANIC & MEDICINAL CHEMISTRY LETTERS 1998, V8(16), P2111 HCAPLUS

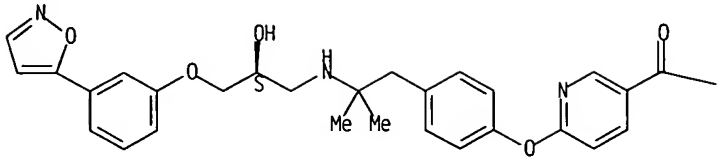
IT **391920-14-2P 391920-78-8P**
RL: PAC (Pharmacological activity): SPN (Synthetic preparation): THU (Therapeutic use): BIOL (Biological study): PREP (Preparation): USES (Uses)
(drug: synthesis and use of heteroaryl-substituted-aryloxyalkylaryl compds. as .beta.3-adrenergic agonists)

RN 391920-14-2 HCAPLUS
CN 3-Pyridinecarboxamide, 6-[4-[2-[[(2S)-2-hydroxy-3-[3-(5-isoxazolyl)phenoxy]propyl]amino]-2-methylpropyl]phenoxy]- (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

PAGE 1-A

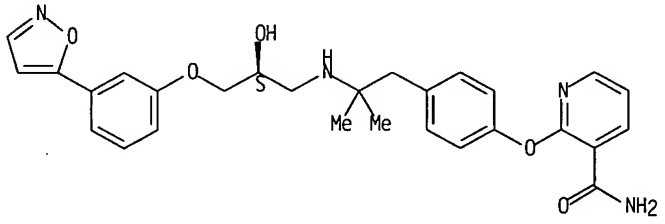


PAGE 1-B

—NH_2

RN 391920-78-8 HCAPLUS
CN 3-Pyridinecarboxamide, 2-[4-[2-[[(2S)-2-hydroxy-3-[3-(5-isoxazolyl)phenoxy]propyl]amino]-2-methylpropyl]phenoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L17 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:653399 HCAPLUS
DN 135:344414
ED Entered STN: 07 Sep 2001
TI Solid-Phase Synthesis of Isoxazoles Using Vinyl Ethers as Chameleon Catches
AU Barrett, Anthony G. M.; Procopiou, Panayiotis A.; Voigtmann, Ulrike
CS Department of Chemistry, Imperial College of Science Technology and Medicine, London, SW7 2AY, UK
SO Organic Letters (2001), 3(20), 3165-3168
CODEN: ORLEF7; ISSN: 1523-7060
PB American Chemical Society
DT Journal
LA English
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 25
OS CASREACT 135:344414
AB Regioselective 1,3-dipolar cycloaddns. of supported vinyl ethers R1C(:CH2)OCH2-polymer, prepared by the Tebbe olefination of R1CO2CH2-polymer, with Et cyanoformate N-oxide gave supported isoxazoline derivs. Release from the support under mild acidic conditions gave the isoxazoles Et 5-R1-isoxazole-3-carboxylates. Alternatively, further on-resin functionalization of the R1 substituent using Suzuki coupling reactions and release from the support under acidic conditions gave more structurally diverse isoxazoles.

ST solid phase synthesis isoxazole; dipolar cycloaddn supported vinyl ether; Suzuki coupling reaction solid phase synthesis isoxazole

IT Cycloaddition reaction
(1,3-dipolar, regioselective; regioselective 1,3-dipolar cycloaddns. of supported vinyl ethers with Et cyanoformate N-oxide)

IT Suzuki coupling reaction
(Suzuki coupling reactions in solid-phase synthesis of isoxazoles)

IT Solid phase synthesis
(regioselective 1,3-dipolar cycloaddns. of supported vinyl ethers with Et cyanoformate N-oxide)

IT **371157-24-3P 371157-25-4P 371157-26-5P**
371157-27-6P 371157-28-7P **371157-29-8P** 371157-30-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Suzuki coupling and regioselective 1,3-dipolar cycloaddns. of supported vinyl ethers with Et cyanoformate N-oxide)

IT 1423-26-3, 3-Trifluoromethylphenylboronic acid 6165-69-1 13331-27-6, 3-Nitrophenylboronic acid 14047-29-1, 4-Carboxyphenylboronic acid 78887-39-5, 3-Acetamidophenylboronic acid 87199-17-5, 4-Formylphenylboronic acid 126747-14-6, 4-Cyanophenylboronic acid
RL: RCT (Reactant); RACT (Reactant or reagent)
(Suzuki coupling reactions of)

IT 230647-85-5P 371157-19-6P 371157-20-9P 371157-21-0P 371157-22-1P 371157-23-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Suzuki coupling reactions of supported vinyl ethers)

IT 14337-43-0, Ethyl chloroximidoacetete 140455-42-1D, polymer supported 215457-53-7D, polymer supported 371157-31-2D, polymer supported 371157-33-4D, polymer supported 371157-34-5D, polymer supported 371157-35-6D, polymer supported 371157-36-7D, polymer supported 371157-37-8D, polymer supported
RL: RCT (Reactant); RACT (Reactant or reagent)
(regioselective 1,3-dipolar cycloaddns. of supported vinyl ethers with Et cyanoformate N-oxide)

IT 33277-15-5P 90924-54-2P 371157-13-0P 371157-14-1P 371157-15-2P 371157-16-3P 371157-17-4P 371157-18-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(regioselective 1,3-dipolar cycloaddns. of supported vinyl ethers with Et cyanoformate N-oxide)

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Ball, C; Chem Commun 1998, P2019 HCAPLUS
(2) Boa, A; J Chem Soc, Perkin Trans 1 1993, P1277 HCAPLUS
(3) Boa, A; J Chem Soc, Perkin Trans 1 1994, P953 HCAPLUS
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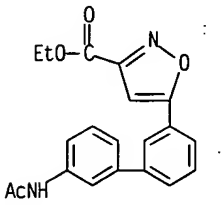
(19) Simoni, D; J Med Chem 2001, V44, P2308 HCAPLUS
(20) Talley, J; J Med Chem 2000, V43, P775 HCAPLUS
(21) Torsell, K; Nitrile Oxides, Nitrones and Nitronates in Organic Synthesis 1988

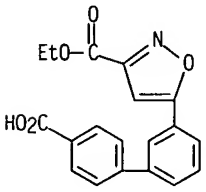
IT **371157-24-3P 371157-25-4P 371157-26-5P**
371157-29-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
(Suzuki coupling and regioselective 1,3-dipolar cycloaddns. of supported vinyl ethers with Et cyanoformate N-oxide)

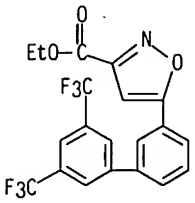
RN 371157-24-3 HCAPLUS
CN 3-Isoxazolecarboxylic acid, 5-[3'-(acetylamino)[1,1'-biphenyl]-3-yl]-, ethyl ester (9CI) (CA INDEX NAME)



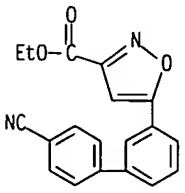
RN 371157-25-4 HCAPLUS
CN 3-Isoxazolecarboxylic acid, 5-(4'-carboxy[1,1'-biphenyl]-3-yl)-, 3-ethyl ester (9CI) (CA INDEX NAME)



RN 371157-26-5 HCAPLUS
CN 3-Isoxazolecarboxylic acid, 5-[3',5'-bis(trifluoromethyl)[1,1'-biphenyl]-3-yl]-, ethyl ester (9CI) (CA INDEX NAME)



RN 371157-29-8 HCAPLUS
CN 3-Isoxazolecarboxylic acid, 5-(4'-cyano[1,1'-biphenyl]-3-yl)-, ethyl ester (9CI) (CA INDEX NAME)



L17 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:581835 HCAPLUS

DN 135:152794
ED Entered STN: 10 Aug 2001
TI Preparation of substituted cyanoacetamide derivatives as herbicides
IN Yamanaka, Hiroyuki; Kajita, Satoshi; Tanaka, Katsunori; Koguchi, Masami; Yamada, Shigeo; Takahashi, Akihiro
PA Nippon Soda Co., Ltd, Japan
SO PCT Int. Appl., 54 pp.
CODEN: PIXXD2
DT Patent
LA Japanese
IC C07C317-24; C07C317-32; A01N041-10; C07D261-08; C07D263-32; C07D277-26; C07D277-22; C07D271-06; C07D271-10; C07D231-12; C07D249-08; C07D257-04; C07D307-38; C07D333-24
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5, 25
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001056979	A1	20010809	WO 2001-JP603	20010130

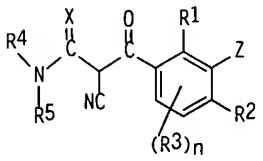
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

PRAI JP 2000-27226 A 20000131
JP 2000-304838 A 20001004

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES		
WO 2001056979	IC	C07C317-24IC	C07C317-32IC	A01N041-10IC
		C07D261-08IC	C07D263-32IC	C07D277-26IC
		C07D277-22IC	C07D271-06IC	C07D271-10IC
		C07D231-12IC	C07D249-08IC	C07D257-04IC
		C07D307-38IC	C07D333-24	

OS MARPAT 135:152794
GI



I

AB The title compds. I [R1 and R2 are each hydrogen, nitro, cyano, halogeno, C1-6 alkyl, C1-6 alkylsulfonyl, or the like; R3 is nitro, cyano, halogeno, C1-6 alkyl, or the like; n is 0, 1 or 2; R4 and R5 are each hydrogen, C1-6 alkyl, C1-6 alkoxy, or the like, or alternatively they may be united to form an alkylene chain, a heterocyclic group, or the like; X is oxygen or sulfur; and Z is formyl, di(C1-6 alkoxy)methyl, Ph, a heterocyclic group, or the like] are prepared 3-(Azetidin-1-yl)-2-[2-methyl-3-(3-methylisoxazol-5-yl)-4-(methylsulfonyl)phenyl]-3-oxopropanenitrile at 250 g/ha gave 80% to 89% control of Abutilon avicennae.
ST cyanoacetamide prepn herbicide; isoxazolmethylsulfonylphenyloxopropanenitrile prepn herbicide

IT Herbicides
(preparation of substituted cyanoacetamide derivs. as herbicides)
IT 353236-70-1P 353236-71-2P 353236-72-3P **353236-73-4P**
353236-74-5P 353236-75-6P 353236-76-7P 353236-77-8P 353236-78-9P
353236-79-0P 353236-80-3P 353236-81-4P 353236-82-5P 353236-83-6P
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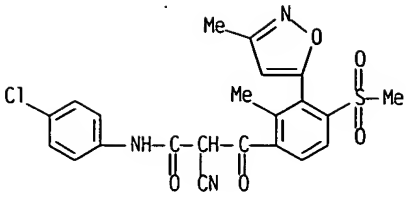
353237-55-5P 353237-56-6P 353237-57-7P 353237-58-8P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted cyanoacetamide derivs. as herbicides)
IT 74-88-4, Methyl iodide, reactions 107-29-9, Acetaldoxime 128-09-6, N-Chlorosuccinimide 530-62-1 540-72-7, Sodium thiocyanate 557-18-6, Diethylmagnesium 630-08-0, Carbon monoxide, reactions 1313-82-2, Sodiumsulfide, reactions 6330-25-2 7391-40-4 7632-00-0, Sodium nitrite 7681-82-5, Sodium iodide, reactions 7726-95-6, Bromine, reactions 13965-03-2, Bis(triphenylphosphine)palladium dichloride 84385-64-8 146561-43-5 196819-96-2 353237-64-6 353237-65-7 353237-66-8 353237-67-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of substituted cyanoacetamide derivs. as herbicides)
IT 345907-82-6P 345907-89-3P 353237-59-9P 353237-60-2P 353237-61-3P 353237-62-4P 353237-63-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of substituted cyanoacetamide derivs. as herbicides)
RE.CNT 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Abbott Laboratories; WO 9424095 A1 1994 HCAPLUS
(2) Ciba-Geigy Ag; JP 02202865 A HCAPLUS
(3) Ciba-Geigy Ag; CA 2004754 A HCAPLUS
(4) Ciba-Geigy Ag; HU 52038 A HCAPLUS
(5) Ciba-Geigy Ag; EP 372470 A2 1990 HCAPLUS
(6) Rohm And Hass Company; US 4781750 A HCAPLUS
(7) Rohm And Hass Company; JP 6284040 A
(8) Rohm And Hass Company; EP 213892 A2 1987 HCAPLUS
(9) Syntex U S A Inc; US 5034410 A 1991 HCAPLUS
IT **353236-73-4P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of substituted cyanoacetamide derivs. as herbicides)
RN 353236-73-4 HCAPLUS
CN Benzenepropanamide, N-(4-chlorophenyl)-.alpha.-cyano-2-methyl-3-(3-methyl-5-isoxazolyl)-4-(methylsulfonyl)-.beta.-oxo- (9CI) (CA INDEX NAME)



L17 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:507532 HCAPLUS
DN 135:107148
ED Entered STN: 13 Jul 2001
TI Preparation of N-cyanomethyl amides as cysteine protease inhibitors
IN Oballa, Renata Marcella; Prasit, Petpiboon; Robichaud, Joel Stephane; Isabel, Elise; Mendonca, Rohan V.; Venkatraman, Shankar; Setti, Eduardo; Wang, Dan-Xiong
PA Merck Frosst Canada & Co., Can.; Axys Pharmaceuticals, Inc.
SO PCT Int. Appl., 157 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM A61K031-40
ICS A61K031-42; A61K031-47; A61K031-50; A61K031-405; C07D209-04; C07D215-00; C07D217-00; C07D235-04; C07D265-30; C07D401-00; C07D405-00; C07D413-00
CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 1, 27, 28, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001049288	A1	20010712	WO 2001-US341	20010105
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2396257	AA	20010712	CA 2001-2396257	20010105
	US 2002052378	A1	20020502	US 2001-754962	20010105
	US 6525036	B2	20030225		
	EP 1248612	A1	20021016	EP 2001-900903	20010105
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
	JP 2003525874	T2	20030902	JP 2001-549656	20010105
PRAI	US 2000-174978P	P	20000106		
	US 2000-256793P	P	20001219		
	WO 2001-US341	W	20010105		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2001049288	ICM	A61K031-40
	ICS	A61K031-42; A61K031-47; A61K031-50; A61K031-405; C07D209-04; C07D215-00; C07D217-00; C07D235-04; C07D265-30; C07D401-00; C07D405-00; C07D413-00
US 2002052378	ECLA	C07C255/25; C07D215/12; C07D239/42B3; C07D263/22; C07D277/36; C07D277/40; C07D277/42; C07D027/48; C07D277/58; C07D277/68; C07D295/14A2; C07D319/18; C07D333/34; C07D417/04+277B+207; C07D071/04+221B+209B;

C07C255/41; C07D207/08A; C07D207/14; C07D209/16; C07D209/30; C07D211/34; C07D213/61

OS MARPAT 135:107148

AB The title compds. R3X1CONHCR1R2CN [I; X1 = CR4R5, CR6R7, NR7 (wherein CR4R5 = (un)substituted cyclohexyl; R6 = H, alkyl; R7 = alkyl, (CH2)1-3 cyclopropyl); R1 = H, alkyl; R2 = H, (un)substituted alkyl; R3 = aryl, cycloalkyl, heterocycloalkyl, etc.] which showed cathepsin B, K, L, and S inhibitory activity (no data), were prepared Thus, reacting 2-(biphenyl-3-yl)-4-methylpentanoic acid (preparation given) with aminoacetonitrile in the presence of PyBOP and Et3N in DMF afforded I [X1 = CH(CH2CHMe2); R1, R2 = H; R3 = 3-biphenyl].

ST amide cyanomethyl prepn formulation cysteine protease cathepsin inhibitor

IT 330474-41-4P 330474-42-5P 349669-22-3P 349669-23-4P 349669-24-5P
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349671-09-6P 349671-10-9P 349671-11-0P 349671-12-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-cyanomethyl amides as protease cysteine inhibitors)

IT 9047-22-7, cathepsin B 37353-41-6, cysteine protease 60616-82-2, cathepsin L 71965-46-3, cathepsin S 94716-09-3, cathepsin K
RL: BSU (Biological study, unclassified); MSC (Miscellaneous); BIOL (Biological study)
(preparation of N-cyanomethyl amides as protease cysteine inhibitors)

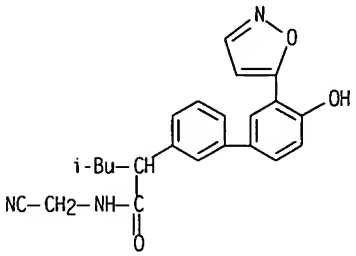
IT 64-04-0, Phenethylamine 70-11-1, 2-Bromo-1-phenylethanone 110-91-8, Morpholine, reactions 701-97-3, 3-Cyclohexylpropanoic acid 1458-98-6, 3-Bromo-2-methylpropene 5292-43-3, tert-Butyl bromoacetate 7352-02-5, Ethyl 2-cyano-4-methylpentanoate 17016-83-0 23948-77-8, [1,1'-Biphenyl]-3-acetic acid 29805-59-2 68819-84-1 349671-24-5 349671-25-6 349671-26-7

RL: RCT (Reactant): RACT (Reactant or reagent)
(preparation of N-cyanomethyl amides as protease cysteine inhibitors)

IT 190661-70-2P 215522-85-3P 349671-13-2P 349671-14-3P 349671-15-4P
349671-16-5P 349671-17-6P 349671-18-7P 349671-19-8P 349671-20-1P
349671-21-2P 349671-22-3P 349671-23-4P
RL: RCT (Reactant): SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of N-cyanomethyl amides as protease cysteine inhibitors)

IT **349669-78-9P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of N-cyanomethyl amides as protease cysteine inhibitors)

RN 349669-78-9 HCAPLUS
CN [1,1'-Biphenyl]-3-acetamide, N-(cyanomethyl)-4'-hydroxy-3'-(5-isoxazolyl)-.alpha.-(2-methylpropyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:300693 HCAPLUS
DN 134:311235
ED Entered STN: 27 Apr 2001
TI Preparation of benzodiazepine derivatives as metabotropic glutamate receptor antagonists
IN Adam, Geo; Alanine, Alexander; Goetschi, Erwin; Mutel, Vincent; Woltering, Thomas Johannes
PA F. Hoffmann-La Roche Ag, Switz.
SO PCT Int. Appl., 142 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D243-00
CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2001029012	A2	20010426	WO 2000-EP9554	20000929
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2386980	AA	20010426	CA 2000-2386980	20000929
BR 2000014761	A	20020702	BR 2000-14761	20000929
EP 1224175	A2	20020724	EP 2000-971302	20000929
EP 1224175	B1	20040317		

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	TR 200201026	T2	20020821	TR 2002-200201026	20000929
	JP 2003512360	T2	20030402	JP 2001-531812	20000929
	AT 261945	E	20040415	AT 2000-971302	20000929
	NZ 518037	A	20040430	NZ 2000-518037	20000929
	ES 2215738	T3	20041016	ES 2000-971302	20000929
	US 6509328	B1	20030121	US 2000-687241	20001013
	ZA 2002002654	A	20030704	ZA 2002-2654	20020404
	NO 2002001691	A	20020410	NO 2002-1691	20020410
	US 2003092677	A1	20030515	US 2002-300449	20021120
PRAI	EP 1999-120519	A	19991015		
	WO 2000-EP9554	W	20000929		
	US 2000-687241	A3	20001013		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2001029012	ICM	C07D243-00
US 6509328	ECLA	C07D243/12; C07D401/04+243+213; C07D403/10+243+233; C07D403/10+249+243; C07D403/10+249B+243; C07D413/10+261+243; C07D413/10+271+243; C07D417/06+277B+243; C07D417/10++277+243
US 2003092677	ECLA	C07D243/12; C07D401/04+243+213; C07D403/10+243+233; C07D403/10+249+243; C07D403/10+249B+243; C07D413/10+261+243; C07D413/10+271+243; C07D417/06+277B+243; C07D417/10++277+243

OS MARPAT 134:311235

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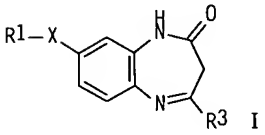

I

AB The title compds. [I; X is a single bond or an ethynediyl group; wherein, in case X is a single bond, R1 is hydrogen, halogen, nitro, lower alkyl, halo-lower alkyl, alkoxycarbonyl, lower cycloalkyl optionally substituted with oxygen, (un)substituted benzoyl or Ph, styrenyl, phenylethyl, naphthyl, biphenyl, benzofuranyl, or (un)substituted 5 or 6 membered heterocyclic ring; wherein in case X is an ethynediyl group, R1 is hydrogen, lower alkyl, optionally substituted with hydroxy, halo-lower alkyl, (un)substituted lower cycloalkyl or lower cycloalkenyl, lower alkenyl, (un)substituted Ph or 5 or 6 membered heterocyclic ring, or benzofuranyl; R3 is (un)substituted Ph, pyridinyl, thiophenyl, thiazolyl, or a 5-membered aromatic heterocycle, with the proviso that, if X is a single bond and R3 is pyridinyl, R1 is not hydrogen, or methyl] and their pharmaceutically acceptable acid addition salts are prepared These compds. can be used for treating or preventing acute and/or chronic neurol. disorders such as psychosis, schizophrenia, Alzheimer's disease, cognitive disorders, and memory deficits. Thus, [2-amino-4-(4-fluorophenylethynyl)phenyl]-carbamic acid tert-Bu ester (preparation given) and 6-(3-imidazol-1-ylphenyl)-2,2-dimethyl-[1,3]dioxin-4-one (preparation given) were refluxed in toluene to give [4-(4-fluorophenylethynyl)-2-[3-(3-imidazol-1-ylphenyl)-3-oxopropionylamino]phenyl]carbamic acid tert-Bu ester which was treated with CF3CO2H in CH2Cl2 to give 8-(4-Fluorophenylethynyl)-4-(3-imidazol-1-ylphenyl)-1,3-dihydrobenzo[b](1,4)diazepin-2-one (II). II showed the antagonism against group II mGlu receptor with Ki of 0.004 .mu.M in an assay using [3H]-LY354740 binding on mGlu2 transfected CHO cell membranes.

ST benzodiazepine prepn metabotropic glutamate receptor antagonist:

benzodiazepinone prepn antipsychotic; schizophrenia treatment
benzodiazepinone prepn; imidazolylphenyldihydrobenzodiazepinone prepn
treatment cognitive disorder; memory deficit benzodiazepinone prepn

IT Mental disorder
(cognitive; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT Cognition
(disorder; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT Alzheimer's disease
Antipsychotics
Schizophrenia
(preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT Memory, biological
(retention defect; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT 4968-94-9P 13422-80-5P 19936-11-9P, N-(4-Cyclopropylphenyl)acetamide
53503-61-0P 139911-29-8P, 4-Fluoro-2-methylphenylboronic acid
178975-04-7P 335254-68-7P, 4-Iodo-2-nitrophenyl isocyanate
335254-69-8P, (4-Iodo-2-nitrophenyl)carbamic acid tert-butyl ester
335254-70-1P, (4-Isopropyl-2-nitrophenyl)carbamic acid tert-butyl ester
335254-71-2P, (4-Cyclopropyl-2-nitrophenyl)carbamic acid tert-butyl ester
335254-73-4P, (4'-Methoxy-3-nitrobiphenyl-4-yl)carbamic acid tert-butyl ester 335254-74-5P 335254-75-6P 335254-76-7P 335254-77-8P
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4-Fluoro-2-methoxymethoxyphenylboronic acid 335254-88-1P 335254-89-2P
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RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT 335257-25-5P 335257-26-6P 335257-27-7P 335257-28-8P 335257-29-9P
335257-30-2P 335257-31-3P **335257-32-4P** 335257-33-5P
335257-34-6P 335257-35-7P 335257-36-8P 335257-37-9P 335257-38-0P
335257-39-1P 335257-40-4P 335257-41-5P **335257-42-6P**
335257-43-7P 335257-44-8P 335257-45-9P 335257-46-0P 335258-91-8P
335259-19-3P 335259-20-6P 335259-22-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT 335257-47-1P 335257-48-2P 335257-49-3P 335257-50-6P 335257-51-7P
335257-52-8P 335257-53-9P 335257-54-0P 335257-56-2P 335257-57-3P
335257-58-4P 335257-59-5P 335257-60-8P 335257-62-0P 335257-63-1P
335257-64-2P 335257-66-4P 335257-67-5P 335257-68-6P 335257-69-7P
335257-70-0P 335257-71-1P 335257-72-2P 335257-73-3P 335257-74-4P
335257-75-5P 335257-76-6P 335257-77-7P 335257-78-8P 335257-79-9P
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335257-85-7P 335257-86-8P 335257-87-9P 335257-88-0P 335257-89-1P
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335258-12-3P 335258-13-4P 335258-14-5P 335258-15-6P 335258-16-7P
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335259-27-3P, 4'-Fluorobiphenyl-3,4-diamine 335259-28-4P 335259-30-8P
335259-31-9P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

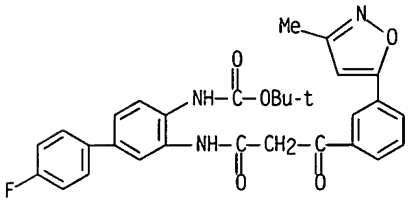
IT 70-23-5, Ethyl bromopyruvate 74-88-4, Methyl iodide, reactions 74-89-5, Methylamine, reactions 78-27-3, 1-Ethynyl-1-cyclohexanol 78-95-5, Chloroacetone 80-73-9, 1,3-Dimethyl-2-imidazolidinone 88-74-4, 2-Nitroaniline 92-66-0, 4-Bromobiphenyl 98-03-3, Thiophene-2-carboxaldehyde 98-09-9, Benzenesulfonyl chloride 98-80-6, Phenylboronic acid 99-05-8, 3-Aminobenzoic acid 106-95-6, Allyl bromide, reactions 107-29-9, Acetaldoxime 107-30-2, Chloromethylmethyl ether 108-22-5, Isopropenyl acetate 109-01-3, N-Methylpiperazine 109-04-6, 2-Bromopyridine 110-91-8, Morpholine, reactions 115-19-5, 2-Methyl-3-butyn-2-ol 121-90-4, 3-Nitrobenzoyl chloride 122-51-0, Triethyl orthoformate 124-63-0, Methanesulfonyl chloride 141-43-5, 2-Aminoethanol, reactions 288-32-4, Imidazole, reactions 348-52-7, 2-Fluoroiodobenzene 352-34-1, 1-Fluoro-4-iodobenzene 452-63-1, 2-Bromo-5-fluorotoluene 503-38-8, Diphosgene 529-28-2, 2-Iodoanisole 536-74-3, Phenylacetylene 540-88-5, tert-Butyl acetate 582-33-2, Ethyl 3-aminobenzoate 615-37-2, 2-Iodotoluene 615-41-8, 1-Chloro-2-iodobenzene 618-46-2, 3-Chlorobenzoyl chloride 623-00-7, 4-Bromobenzonitrile 624-31-7, 4-Iodotoluene 625-95-6, 3-Iodotoluene 626-55-1, 3-Bromopyridine 637-87-6, 1-Chloro-4-iodobenzene 638-07-3, Ethyl 4-chloro-3-oxobutanoate 645-36-3, Aminoacetaldehyde diethyl acetal 768-35-4, 3-Fluorophenylboronic acid 768-60-5, 4-Methoxyphenylacetylene 813-19-4, Hexabutyldistannane 873-31-4, 2-Chlorophenylacetylene 873-73-4, 4-Chlorophenylacetylene 1066-54-2, Trimethylsilylacetylene 1076-38-6, 4-Hydroxycoumarin 1120-87-2, 4-Bromopyridine 1122-54-9, 4-Acetylpyridine 1711-05-3, 3-Methoxybenzoyl chloride 1711-10-0, 3-Iodobenzoyl chloride 1711-11-1, 3-Cyanobenzoyl chloride 1765-93-1, 4-Fluorophenylboronic acid 1993-03-9, 2-Fluorophenylboronic acid 2131-63-7, 3-Isothiocyanatobenzoic acid 2208-07-3, Ethyl acetimidate hydrochloride 2251-65-2, 3-Trifluoromethylbenzoyl chloride 2265-93-2, 2,4-Difluoro-1-iodobenzene 3034-53-5, 2-Bromothiazole 3282-30-2, Pivaloyl chloride 3385-94-2, Hexamethyldisilthiane 3437-95-4, 2-Iodothiophene 4298-52-6, 2-Ethynylthiophene 5271-67-0, Thiophene-2-carbonyl chloride 5398-36-7, Ethyl 2-amino-4-thiazolecarboxylate 5720-07-0, 4-Methoxyphenylboronic acid 6148-64-7, Ethyl malonate potassium salt 6165-69-1, Thiophene-3-boronic acid 7803-49-8, Hydroxylamine, reactions 7803-57-8, Hydrazine hydrate 10365-98-7, 3-Methoxyphenylboronic acid 13331-23-2, Furan-2-boronic acid 13531-48-1, Methyl 3-cyanobenzoate 13922-41-3, 1-Naphthylboronic acid 14171-36-9, Magnesium methyl carbonate 18457-04-0, Bis(trimethylsilyl)malonate 20555-91-3, 3,4-Dichloroiodobenzene 22059-22-9, N-Hydroxyacetamidine 37595-74-7 39986-42-0, 3-Azidobenzoyl chloride 53090-46-3 53547-61-8, Vinyl triflate 55552-70-0, Furan-3-boronic acid 57385-16-7, 4-Ethynyltetrahydropyran-4-ol 57390-38-2, 2-Aminopropionaldehyde dimethyl acetal 58481-14-4, 2-Cyano-isonicotinic acid ethyl ester 63139-21-9, 4-Ethylphenylboronic acid 63649-64-9, 4-Isopropyl-2-nitroaniline 67808-35-9 69931-93-7, 3-Oxo-3-(thiophen-2-yl)propionic acid 75486-33-8 78495-63-3, 2-Fluoro-6-methoxyphenylboronic acid 79099-07-3, N-tert-Butoxycarbonyl-4-piperidone 86270-03-3, 3-Trifluoromethoxybenzoyl chloride 86427-02-3, 3-Chlorothiophene-2-carbonyl chloride 93066-93-4, Methyl 3-azidobenzoate 98437-24-2 103962-05-6, 1-Iodo-4-(trifluoromethoxy)benzene 108035-47-8, 3-(1H-Imidazol-1-yl)benzoic acid 121219-16-7, 2,3-Difluorophenylboronic acid 139301-27-2, 4-(Trifluoromethoxy)phenylboronic acid 144025-03-6, 2,4-

Difluorophenylboronic acid 162269-78-5 167626-27-9 168422-44-4
177984-28-0 178742-95-5, Ethyl 3-ethynylbenzoate 188881-22-3
193353-34-3, 2,5-Difluorophenylboronic acid 204196-80-5,
3-(Tetrazol-1-yl)benzoic acid 256420-32-3, Ethyl 2-(imidazol-1-
yl)thiazole-4-carboxylate 295349-62-1 335256-00-3 335256-16-1,
2-Isothiocyanato-1,1-dimethoxypropane 335256-20-7 335256-22-9
335256-23-0, 3-Cyanothiophene-2-carbonyl chloride 335256-36-5,
3-(1H-Imidazol-1-yl)benzoyl chloride hydrochloride 335256-53-6
335259-29-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

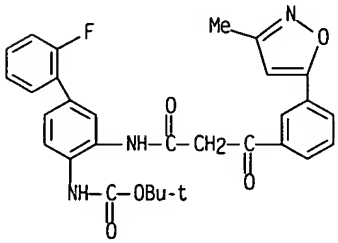
IT 20691-72-9P, 4-Iodo-2-nitroaniline 138647-49-1P 335254-72-3P,
4-Cyclopropyl-2-nitrophenylamine 335255-80-6P 335255-92-0P, Ethyl
3-(2-methylimidazol-1-yl)benzoate 335255-95-3P 335257-95-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reactant; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT **335257-32-4P 335257-42-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

RN 335257-32-4 HCAPLUS
CN Carbamic acid, [4'-fluoro-3-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino][1,1'-biphenyl]-4-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



RN 335257-42-6 HCAPLUS
CN Carbamic acid, [2'-fluoro-3-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino][1,1'-biphenyl]-4-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L17 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2001:300692 HCAPLUS
DN 134:311234

ED Entered STN: 27 Apr 2001
TI Preparation of benzodiazepine derivatives as metabotropic glutamate receptor antagonists
IN Adam, Geo; Alanine, Alexander; Goetschi, Erwin; Mutel, Vincent; Woltering, Thomas Johannes
PA F. Hoffmann-La Roche Ag, Switz.
SO PCT Int. Appl., 140 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D243-00
CC 28-21 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1

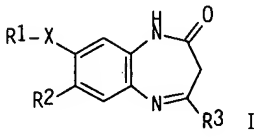
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001029011	A2	20010426	WO 2000-EP9553	20000929
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2386974	AA	20010426	CA 2000-2386974	20000929
	BR 2000014859	A	20020716	BR 2000-14859	20000929
	EP 1224174	A2	20020724	EP 2000-969347	20000929
	EP 1224174	B1	20030917		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	TR 200201023	T2	20020923	TR 2002-200201023	20000929
	JP 2003512359	T2	20030402	JP 2001-531811	20000929
	AT 250039	E	20031015	AT 2000-969347	20000929
	PT 1224174	T	20040130	PT 2000-969347	20000929
	ES 2204704	T3	20040501	ES 2000-969347	20000929
	AU 774451	B2	20040624	AU 2000-79102	20000929
	NZ 517999	A	20040730	NZ 2000-517999	20000929
	US 6407094	B1	20020618	US 2000-687240	20001013
	ZA 2002002544	A	20030630	ZA 2002-2544	20020328
	NO 2002001690	A	20020410	NO 2002-1690	20020410
PRAI	EP 1999-120520	A	19991015		
	WO 2000-EP9553	W	20000929		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 2001029011	ICM	C07D243-00
US 6407094	ECLA	C07D243/12

OS MARPAT 134:311234
GI



I

AB The title compds. [I; X is a single bond or an ethynediyl group; wherein, in case X is a single bond, R1 is halogen or (un)substituted phenyl; in case X is an ethynediyl group, R1 is (un)substituted phenyl; R2 is

halogen, hydroxy, lower alkyl, lower haloalkyl, lower alkoxy, hydroxymethyl, hydroxyethoxy, lower alkoxy(ethoxy)n (n = 1 to 4), lower alkoxymethyl, cyanomethoxy, morpholin-4-yl, thiomorpholin-4-yl, 1-oxothiomorpholin-4-yl, 1,1-dioxothiomorpholin-4-yl, 4-oxopiperidin-1-yl, 4-alkoxypiperidin-1-yl, 4-hydroxypiperidine-1-yl, 4-hydroxyethoxypiperidin-1-yl, 4-lower alkylpiperazine-1-yl, alkoxycarbonyl, 2-dialkylaminoethylthio, N,N-bis(lower alkyl)amino-lower alkyl, carbamoylmethyl, alkylsulfonyl, etc.; R3 is (un)substituted 5 or 6 membered aryl or heteroaryl, etc.] and their pharmaceutically acceptable addition salts are prepared These compds. can be used for treating or preventing acute and/or chronic neurol. disorders such as psychosis, schizophrenia, Alzheimer's disease, cognitive disorders and memory deficits. Thus, a mixture of (5-amino-2-tert-butoxy-2',5'-difluorobiphenyl-4-yl)carbamic acid tert-Bu ester and 3-(2,2-dimethyl-6-oxo-6H-[1,3]dioxin-4-yl)benzonitrile in toluene was refluxed to give [2-tert-butoxy-5-[[3-(3-cyanophenyl)-3-oxo-propionyl]amino]-2',5'-difluorobiphenyl-4-yl]carbamic acid tert-Bu ester which was treated with CF3CO2H in CH2Cl2 to give 3-[7-(2,5-Difluorophenyl)-8-hydroxy-4-oxo-4,5-dihydro-3H-benzo[b](1,4)diazepin-2-yl]benzonitrile (II). II in vitro inhibited the binding of [3H]-LY354740 binding on mGlu2 receptor transfected CHO cell membranes with Ki of 0.006 .mu.M.

ST benzodiazepine prepn metabotropic glutamate receptor antagonist; psychosis treatment benzodiazepine; schizophrenia treatment benzodiazepine; Alzheimer disease treatment benzodiazepine; cognitive disorder treatment benzodiazepine; memory deficit treatment benzodiazepine 2134

IT Mental disorder
(cognitive; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT Cognition
(disorder; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT Glutamate antagonists
(metabotropic glutamate receptor; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT Alzheimer's disease
Antipsychotics
Schizophrenia
(preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT Memory, biological
(retention defect; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT 4968-94-9P 5398-36-7P, Ethyl 2-amino-4-thiazolecarboxylate 6968-22-5P, 3-Amino-4-nitrobenzoic acid 13422-80-5P 53503-61-0P 69931-93-7P 178975-04-7P 335254-68-7P, 4-Iodo-2-nitrophenyl isocyanate 335254-69-8P, (4-Iodo-2-nitrophenyl)carbamic acid tert-butyl ester 335255-09-9P 335255-80-6P 335255-81-7P 335255-83-9P 335255-84-0P 335255-86-2P 335255-87-3P 335255-88-4P 335255-89-5P 335255-90-8P 335255-91-9P 335255-92-0P 335255-93-1P 335255-94-2P 335255-95-3P 335255-96-4P 335255-97-5P 335255-98-6P 335255-99-7P 335256-01-4P 335256-02-5P 335256-03-6P 335256-05-8P 335256-06-9P 335256-07-0P 335256-08-1P 335256-12-7P, 5-Cyano-2-fluorobenzoyl chloride 335256-13-8P 335256-14-9P 335256-15-0P 335256-17-2P 335256-18-3P 335256-19-4P 335256-20-7P 335256-21-8P 335256-22-9P 335256-24-1P 335256-25-2P 335256-26-3P 335256-27-4P 335256-28-5P 335256-29-6P 335256-30-9P 335256-31-0P 335256-32-1P 335256-33-2P 335256-35-4P 335256-37-6P 335256-39-8P 335256-40-1P 335256-41-2P 335256-42-3P 335256-43-4P 335256-44-5P 335349-56-9P 335349-57-0P, 5-Chloro-4-iodo-2-nitrophenylamine 335349-58-1P, 4-Iodo-5-methyl-2-

nitrophenylamine 335349-59-2P, 5-Amino-2-iodo-4-nitrobenzoic acid methyl ester 335349-60-5P 335349-61-6P 335349-62-7P 335349-63-8P 335349-64-9P 335349-65-0P 335349-66-1P, 4-Iodo-5-methoxy-2-nitrophenylamine 335349-67-2P 335349-68-3P, 4-Iodo-5-(2-methoxyethoxy)-2-nitrophenylamine 335349-69-4P 335349-70-7P 335349-71-8P 335349-72-9P 335349-73-0P 335349-74-1P, (5-Amino-2-iodo-4-nitrophenyl)acetonitrile 335349-75-2P 335349-76-3P 335349-77-4P 335349-78-5P 335349-79-6P 335349-80-9P 335349-81-0P 335349-82-1P 335349-83-2P 335349-84-3P, [5-[(2-Hydroxyethyl)methylamino]-4-iodo-2-nitrophenyl]-carbamic acid tert-butyl ester 335349-85-4P 335349-86-5P 335349-87-6P 335349-88-7P 335349-89-8P 335349-90-1P 335349-91-2P 335349-92-3P 335349-93-4P 335349-94-5P 335349-95-6P 335349-96-7P 335349-97-8P 335349-98-9P 335349-99-0P 335350-00-0P 335350-01-1P, (2-Chloro-5-nitrobiphenyl-4-yl)carbamic acid tert-butyl ester 335350-02-2P, (2-Methyl-5-nitrobiphenyl-4-yl)carbamic acid tert-butyl ester 335350-03-3P 335350-04-4P 335350-05-5P 335350-06-6P 335350-07-7P 335350-08-8P 335350-09-9P, (5-Cyanomethoxy-4-iodo-2-nitrophenyl)carbamic acid tert-butyl ester 335350-10-2P 335350-11-3P 335350-12-4P 335350-13-5P 335350-14-6P 335350-15-7P 335350-16-8P 335350-17-9P 335350-18-0P 335350-19-1P 335350-20-4P 335350-21-5P 335350-22-6P 335350-23-7P 335350-24-8P 335350-25-9P 335350-26-0P 335350-27-1P 335350-28-2P 335350-29-3P 335350-30-6P 335350-31-7P 335350-32-8P 335350-33-9P 335350-34-0P 335350-35-1P 335350-36-2P 335350-37-3P 335350-38-4P 335350-39-5P 335350-40-8P 335350-41-9P 335350-42-0P 335350-43-1P 335350-44-2P 335350-45-3P 335350-46-4P 335350-47-5P 335350-48-6P 335350-49-7P 335350-50-0P 335350-51-1P 335350-52-2P 335350-54-4P 335350-55-5P 335350-56-6P 335350-57-7P 335350-58-8P 335350-59-9P 335350-60-2P 335350-61-3P 335350-62-4P 335350-63-5P 335350-64-6P 335350-65-7P 335350-66-8P 335350-67-9P 335350-68-0P 335350-69-1P 335350-70-4P 335350-71-5P 335350-72-6P 335350-73-7P 335350-74-8P 335350-75-9P 335350-76-0P 335350-77-1P 335350-78-2P 335350-79-3P 335350-80-6P 335350-81-7P 335350-82-8P 335350-83-9P 335350-84-0P 335350-85-1P 335350-86-2P 335350-87-3P 335350-88-4P 335350-89-5P 335350-90-8P 335350-91-9P 335350-92-0P 335350-93-1P 335350-94-2P 335350-95-3P 335350-96-4P 335350-97-5P 335350-98-6P 335350-99-7P 335351-00-3P 335351-01-4P 335351-02-5P 335351-03-6P 335351-04-7P 335351-05-8P 335351-06-9P 335351-07-0P 335351-08-1P 335351-09-2P 335351-10-5P 335351-11-6P 335351-12-7P 335351-13-8P 335351-14-9P 335351-15-0P 335351-16-1P 335351-17-2P 335351-18-3P 335351-19-4P 335351-20-7P 335351-21-8P 335351-22-9P 335351-23-0P 335351-24-1P 335351-25-2P 335351-26-3P 335351-27-4P 335351-29-6P 335351-30-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT 335351-32-1P 335351-33-2P 335351-34-3P 335351-35-4P 335351-36-5P 335351-37-6P 335351-38-7P 335351-39-8P 335351-40-1P 335351-41-2P 335351-42-3P 335351-43-4P 335351-44-5P 335351-45-6P 335351-46-7P 335351-47-8P 335351-48-9P 335351-49-0P 335351-50-3P 335351-51-4P 335351-52-5P 335351-53-6P 335351-54-7P 335351-55-8P 335351-56-9P 335351-57-0P 335351-58-1P 335351-59-2P 335351-60-5P 335351-61-6P 335351-62-7P 335351-63-8P 335351-64-9P 335351-65-0P 335351-66-1P 335351-68-3P 335351-69-4P 335351-70-7P 335351-71-8P 335351-72-9P 335351-73-0P 335351-74-1P 335351-75-2P 335351-76-3P 335351-77-4P 335351-78-5P 335351-79-6P 335351-80-9P 335351-81-0P 335351-82-1P 335351-83-2P 335351-84-3P 335351-85-4P 335351-86-5P 335351-87-6P 335351-88-7P 335351-89-8P 335351-90-1P 335351-91-2P 335351-92-3P 335351-93-4P 335351-94-5P 335351-95-6P 335351-96-7P 335351-97-8P 335351-98-9P 335351-99-0P 335352-00-6P 335352-01-7P 335352-02-8P **335352-03-9P** 335352-04-0P 335352-05-1P 335352-06-2P 335352-07-3P, (5-Hydroxy-2-nitrophenyl)carbamic acid tert-butyl ester 335352-09-5P, (5-Hydroxy-4-iodo-2-nitrophenyl)carbamic acid tert-butyl

ester
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT 335256-34-3P 335351-31-0P 335352-21-1P 335352-31-3P 335352-34-6P
335352-58-4P 335352-63-1P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT 335258-57-6P 335352-10-8P 335352-11-9P 335352-12-0P 335352-13-1P
335352-14-2P 335352-15-3P 335352-16-4P 335352-17-5P 335352-18-6P
335352-19-7P 335352-20-0P 335352-22-2P 335352-23-3P 335352-24-4P
335352-25-5P 335352-26-6P 335352-27-7P 335352-28-8P 335352-29-9P
335352-30-2P 335352-32-4P 335352-33-5P 335352-35-7P 335352-36-8P
335352-37-9P 335352-38-0P 335352-39-1P 335352-40-4P 335352-41-5P
335352-42-6P 335352-43-7P 335352-44-8P 335352-45-9P 335352-46-0P
335352-47-1P 335352-48-2P 335352-49-3P 335352-50-6P 335352-51-7P
335352-52-8P 335352-53-9P 335352-54-0P 335352-55-1P 335352-56-2P
335352-57-3P 335352-59-5P 335352-60-8P 335352-61-9P 335352-62-0P
335352-64-2P 335352-65-3P 335352-66-4P 335352-67-5P 335352-68-6P
335352-69-7P 335352-70-0P 335352-71-1P 335352-72-2P 335352-73-3P
335352-74-4P 335352-75-5P 335352-76-6P 335352-77-7P 335352-78-8P
335352-79-9P 335352-80-2P 335352-81-3P 335352-82-4P 335352-83-5P
335352-84-6P 335352-85-7P 335352-86-8P 335352-88-0P 335352-89-1P
335352-90-4P 335352-91-5P 335352-92-6P 335352-93-7P 335352-94-8P
335352-95-9P 335352-96-0P 335352-97-1P 335352-98-2P 335352-99-3P
335353-00-9P 335353-01-0P 335353-02-1P 335353-04-3P 335353-05-4P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT 335353-03-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT 67-56-1, Methanol, reactions 74-88-4, Methyl iodide, reactions
75-64-9, tert-Butylamine, reactions 77-76-9, 2,2-Dimethoxypropane
79-22-1, Methyl chloroformate 79-37-8, Oxalyl chloride 98-80-6,
Phenylboronic acid 99-05-8, 3-Aminobenzoic acid 100-79-8,
1,2-Isopropylideneglycerol 105-13-5, 4-Methoxybenzyl alcohol 105-56-6,
Ethyl cyanoacetate 107-18-6, Allyl alcohol, reactions 107-29-9,
Acetaldoxime 107-30-2, Chloromethyl methyl ether 108-22-5, Isopropenyl
acetate 108-59-8, Dimethyl malonate 109-01-3, 1-Methylpiperazine
109-83-1, 2-Methylaminoethanol 109-86-4, 2-Methoxyethanol 109-96-6,
3-Pyrroline 110-87-2, 3,4-Dihydro-2H-pyran 110-91-8, Morpholine,
reactions 121-90-4, 3-Nitrobenzoyl chloride 122-51-0, Triethyl
orthoformate 123-75-1, Pyrrolidine, reactions 123-90-0, Thiomorpholine
124-63-0, Methanesulfonyl chloride 141-43-5, Ethanolamine, reactions
177-11-7, 1,4-Dioxa-8-azaspiro[4.5]decane 288-32-4, Imidazole, reactions
503-38-8, Diphosgene 530-62-1, 1,1'-Carbonyldiimidazole 536-74-3,
Phenylacetylene 540-88-5, tert-Butyl acetate 578-46-1,
5-Methyl-2-nitroaniline 582-33-2, Ethyl 3-aminobenzoate 590-17-0,
Bromoacetonitrile 618-46-2, 3-Chlorobenzoyl chloride 619-14-7,
3-Hydroxy-4-nitrobenzoic acid 645-36-3, Aminoacetaldehyde diethyl acetal
766-98-3, 4-Fluorophenylacetylene 813-19-4, Hexabutyldistannane

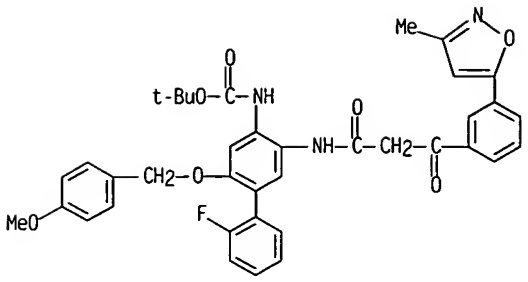
1066-54-2, Trimethylsilylacetylene 1122-54-9, 4-Acetylpyridine
1635-61-6, 5-Chloro-2-nitroaniline 1711-05-3, 3-Methoxybenzoyl chloride
1711-10-0, 3-Iodobenzoyl chloride 1711-11-1, 3-Cyanobenzoyl chloride
1765-93-1, 4-Fluorophenylboronic acid 1993-03-9, 2-Fluorophenylboronic
acid 2131-63-7, 3-Isothiocyanatobenzoic acid 2208-07-3, Ethyl
acetimidate hydrochloride 2251-65-2, 3-Trifluoromethylbenzoyl chloride
2365-48-2, Methyl thioglycolate 3282-30-2, Pivaloyl chloride
4045-24-3, 4-Methoxypiperidine 5271-67-0, Thiophene-2-carbonyl chloride
5292-43-3, tert-Butyl bromoacetate 5382-16-1, 4-Hydroxypiperidine
6148-64-7, Ethyl malonate potassium salt 7580-85-0, 2-tert-Butoxyethanol
7704-34-9, Sulfur, reactions 7803-57-8, Hydrazine hydrate 13242-44-9,
2-Dimethylaminoethanethiol hydrochloride 13531-48-1, Methyl
3-cyanobenzoate 14171-36-9, Magnesium methyl carbonate 17739-45-6,
2-(2-Bromoethoxy)tetrahydro-2H-pyran 18457-04-0,
Bis(trimethylsilyl)malonate 20691-72-9, 4-Iodo-2-nitroaniline
23783-42-8, Tetra(ethylene glycol) monomethyl ether 31938-11-1,
O-Tritylhydroxylamine 36805-97-7, N,N-Dimethylformamide di-tert-butyl
acetal 40256-14-2, 4-(2-Hydroxyethoxy)piperidine 53547-61-8, Vinyl
triflate 57390-38-2, 2-Aminopropionaldehyde dimethyl acetal
58481-14-4, 2-Cyanoisonicotinic acid ethyl ester 67808-35-9 75486-33-8
86270-03-3, 3-Trifluoromethoxybenzoyl chloride 86427-02-3,
3-Chlorothiophene-2-carbonyl chloride 93066-93-4, Methyl 3-azidobenzoate
99512-09-1, 3-Amino-4-nitrobenzoic acid methyl ester 104706-47-0,
(R)-3-Hydroxypyrrolidine hydrochloride 108035-47-8, 3-(1H-Imidazol-1-
yl)benzoic acid 139911-29-8, 4-Fluoro-2-methylphenylboronic acid
167626-27-9 168422-44-4 178742-95-5, Ethyl 3-ethynylbenzoate
193353-34-3, 2,5-Difluorophenylboronic acid 204196-80-5 256420-32-3
295349-62-1, 2-Chloroisonicotinic acid tert-butyl ester 335255-82-8
335256-00-3 335256-16-1, 2-Isothiocyanato-1,1-dimethoxypropane
335256-23-0, 3-Cyanothiophene-2-carbonyl chloride 335256-36-5,
3-(1H-Imidazol-1-yl)benzoyl chloride hydrochloride 335257-58-4
335352-08-4, (5-Allyloxy-2-nitrophenyl)carbamic acid tert-butyl ester
RL: RCT (Reactant); RACT (Reactant or reagent)
(reactant; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

IT 335255-85-1P, Methyl 3-(1H-imidazol-1-yl)benzoate 335256-04-7P, Ethyl 3-(3-methylisoxazol-5-yl)benzoate 335350-53-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(reactant; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

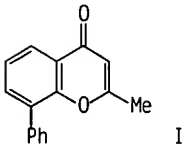
IT **335352-03-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; preparation of benzodiazepine derivs. as metabotropic glutamate receptor antagonists for treating or preventing acute and/or chronic neurol. disorders)

RN 335352-03-9 HCAPLUS

CN Carbamic acid, [2'-fluoro-2-[(4-methoxyphenyl)methoxy]-5-[[3-[3-(3-methyl-5-isoxazolyl)phenyl]-1,3-dioxopropyl]amino][1,1'-biphenyl]-4-yl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)



L17 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1994:409103 HCAPLUS
DN 121:9103
ED Entered STN: 09 Jul 1994
TI Reactions with 2-methyl-8-phenylbenzopyran-4-one and its derivatives
AU Soliman, A. Y.; Mahmoud, M. R.; Madkour, Hassan M. F.
CS Chem. Dep., Fac. Educ., El-Fayoum, Egypt
SO Revue Roumaine de Chimie (1993), 38(9), 1117-25
CODEN: RRCHAX; ISSN: 0035-3930
DT Journal
LA English
CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
GI



I

AB 2-Methyl-8-phenylbenzopyran-4-one (I) was prepared by reaction of 2-hydroxybiphenyl with Et acetoacetate in the presence of concentrated sulfuric acid. The reactivity of I and other chromone derivs. with different nucleophilic reagents was investigated. The IR, 1H NMR and mass spectra of the products are discussed.

ST benzopyranone methylphenyl prepn reaction; isoxazole hydroxyaryl; pyrazole hydroxyaryl; benzopyranol deriv; benzopyranthione deriv

IT Ring closure and formation
(of biphenylol with Et acetoacetate)

IT 104-92-7, p-Bromoanisole 108-85-0, Bromocyclohexane 108-86-1, Bromobenzene, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Grignard reaction of, with methylphenylbenzopyranone)

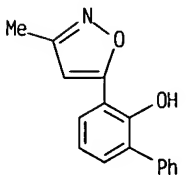
IT 90-43-7, 2-Biphenylol
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization reaction of, with Et acetoacetate)

IT 141-97-9, Ethyl acetoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization reaction of, with biphenylol)

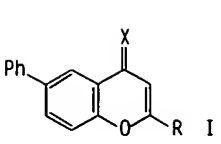
IT 155375-21-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrolysis of)

IT 155375-17-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

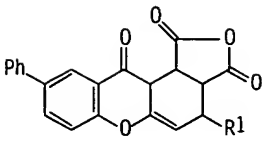
(Reactant or reagent)
(preparation and reaction with hydrazines)
IT 155374-96-2P 155375-11-4P 155375-18-1P
RL: RCT (Reactant): SPN (Synthetic preparation): PREP (Preparation): RACT
(Reactant or reagent)
(preparation and reactions of)
IT 155374-97-3P 155374-98-4P 155374-99-5P **155375-00-1P**
155375-01-2P 155375-02-3P 155375-03-4P 155375-04-5P 155375-05-6P
155375-06-7P 155375-07-8P 155375-08-9P 155375-09-0P 155375-10-3P
155375-12-5P 155375-13-6P 155375-14-7P 155375-15-8P 155375-16-9P
155375-19-2P 155375-20-5P
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of)
IT 108-31-6, Maleic anhydride, reactions
RL: RCT (Reactant): RACT (Reactant or reagent)
(reaction of, with benzopyranone derivative)
IT 57-56-7, Semicarbazide 60-09-3, p-Aminoazobenzene 88-74-4,
2-Nitroaniline 90-02-8, Salicylaldehyde, reactions 100-16-3,
(p-Nitrophenyl)hydrazine 100-46-9, Benzylamine, reactions 100-63-0,
Phenylhydrazine 104-55-2, Cinnamaldehyde 134-32-7, 1-Naphthylamine
135-02-4, o-Anisaldehyde 302-01-2, Hydrazine, reactions 504-29-0,
2-Aminopyridine 552-89-6, o-Nitrobenzaldehyde 587-04-2,
m-Chlorobenzaldehyde 1314-80-3, Diphosphorus pentasulfide 5470-11-1,
Hydroxylamine hydrochloride
RL: RCT (Reactant): RACT (Reactant or reagent)
(reaction of, with methylphenylbenzopyranone)
IT **155375-00-1P**
RL: SPN (Synthetic preparation): PREP (Preparation)
(preparation of)
RN 155375-00-1 HCAPLUS
CN [1,1'-Biphenyl]-2-ol, 3-(3-methyl-5-isoxazolyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1991:6228 HCAPLUS
DN 114:6228
ED Entered STN: 12 Jan 1991
TI Chromones and xanthone derivatives
AU Mahmoud, M. R.; Soliman, A. Y.; Bakeer, H. M.
CS Fac. Sci., Ain Shams Univ., Cairo, Egypt
SO Phosphorus, Sulfur and Silicon and the Related Elements (1990), 53(1-4), 135-43
CODEN: PSSLEC; ISSN: 1042-6507
DT Journal
LA English
CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
OS CASREACT 114:6228
GI



I



II

AB Reaction of chromone I (R = Me, X = O) with R1CHO (R1 = Ph, 4-Me2NC6H4, PhCH:CH) gave I (R = CH:CHR1, X = O) Diels-Alder reactions of the latter with maleic anhydride gave xanthones II (R1 as above). Various reactions of I (R = Me, X = O, S) and II (R1 = CH:CHPh) with R2NHNH2 (R2 = H, Ph), primary aromatic amines and Grignard reagents are reported.

ST chromone deriv reaction; xanthone deriv; styrylchromone Diels Alder maleic anhydride

IT 108-31-6, Maleic anhydride, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Diels-Alder reactions of, with styrylchromones)

IT 92-69-3, 4-Hydroxybiphenyl
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with Et acetoacetate)

IT 141-97-9, Ethyl acetoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclocondensation of, with hydroxybiphenyl, chromone derivative from)

IT 130788-73-7P 130788-74-8P 130788-75-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Diels-Alder reaction of, with maleic anhydride)

IT 58555-03-6P 130788-72-6P 130788-78-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reactions of)

IT 130788-76-0P 130788-77-1P 130788-79-3P 130788-80-6P 130788-81-7P
130788-82-8P 130788-83-9P 130788-84-0P 130788-85-1P 130788-86-2P
130788-87-3P 130788-88-4P 130788-89-5P 130788-90-8P
130788-91-9P 130788-92-0P 130788-93-1P 130788-94-2P 130788-95-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

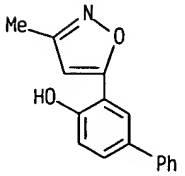
IT 100-63-0, Phenylhydrazine 106-47-8, p-Chloroaniline, reactions
134-32-7, .alpha.-Naphthylamine 917-64-6, Methylmagnesium iodide
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with chromone and xanthone derivs.)

IT 100-10-7, p-(Dimethylamino)benzaldehyde 100-52-7, Benzaldehyde, reactions 104-55-2, Cinnamaldehyde
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methylchromone derivs.)

IT **130788-87-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 130788-87-3 HCAPLUS

CN [1,1'-Biphenyl]-4-ol, 3-(3-methyl-5-isoxazolyl)- (9CI) (CA INDEX NAME)



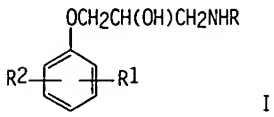
L17 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1982:162685 HCAPLUS
DN 96:162685
ED Entered STN: 12 May 1984
TI Isoxazolyl(aminopropoxy)benzenes
PA Shionogi and Co., Ltd., Japan
SO Jpn. Kokai Tokkyo Koho, 8 pp.
CODEN: JKXXAF
DT Patent
LA Japanese
IC C07D261-08
ICA A61K031-42
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI JP 57024375	A2	19820208	JP 1980-100325	19800721
PRAI JP 1980-100325	A	19800721		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
JP 57024375	IC	C07D261-08
	ICA	A61K031-42

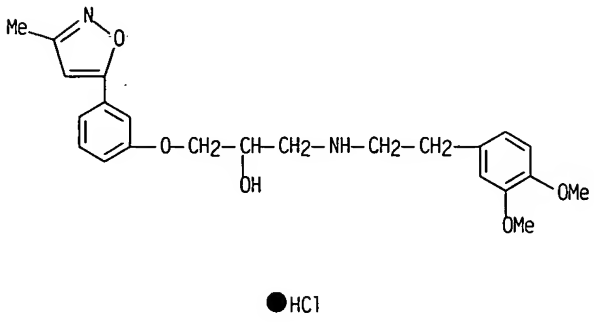
OS CASREACT 96:162685
GI



I

AB I [R = alkyl, substituted phenylalkyl, (cyano)phenoxyalkyl; R1 = substituted isoxazolyl; R2 = H, halo, alkyl, alkanoyl, alkanoylamino, cycloalkylureido, H2NSO2] were prepared Thus, 0.2 g 2-isoxazol-3-yl-4-acetamido-1-(2,3-epoxypropoxy)benzene, prepared from 2-isoxazol-3-yl-4-acetamidophenol and epibromohydrin, reacted with 1 mL Me2CHNH2 in MeOH at 100.degree. for 1 h to give 0.18 g 2-isoxazol-3-yl-4-acetamido-1-[2-hydroxy-3-(isopropylamino)propoxy]benzene. Data for the .beta.-sympatholytic activity of I were tabulated.
ST beta sympatholytic isoxazolylaminopropoxybenzene; amination epoxypropoxybenzene alkylamine
IT Amination
(of (epoxypropoxy)benzene derivs.)
IT Sympatholytics
(.beta.-, (aminopropoxy)isoxazolylbenzenes)
IT 75-31-0, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of (epoxypropoxy)benzene derivative)
IT 81461-35-0P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and amination with isopropylamine)
IT 81460-81-3P 81460-82-4P 81460-83-5P 81460-84-6P 81460-86-8P
81460-87-9P 81460-88-0P 81460-89-1P 81460-90-4P 81460-91-5P
81460-93-7P 81460-95-9P 81460-96-0P 81460-97-1P 81460-98-2P
81461-00-9P 81461-01-0P 81461-03-2P 81461-04-3P 81461-05-4P
81461-06-5P 81461-07-6P 81461-08-7P 81461-09-8P 81461-11-2P
81461-12-3P 81461-14-5P 81461-15-6P 81461-16-7P 81461-17-8P
81461-18-9P 81461-19-0P 81461-20-3P 81461-21-4P 81461-22-5P
81461-23-6P 81461-24-7P 81461-25-8P 81461-26-9P 81461-27-0P
81461-28-1P 81461-29-2P 81461-30-5P 81461-31-6P 81461-32-7P

81461-33-8P **81461-34-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and .beta.-sympatholytic activity of)
IT 3132-64-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with acetamidoisoxazolylphenol)
IT 81461-36-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with epibromohydrin)
IT **81461-34-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and .beta.-sympatholytic activity of)
RN 81461-34-9 HCAPLUS
CN 2-Propanol, 1-[[2-(3,4-dimethoxyphenyl)ethyl]amino]-3-[3-(3-methyl-5-isoxazolyl)phenoxy]-, monohydrochloride (9CI) (CA INDEX NAME)



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